

# Eigenvalue stratification and minimal smooth scaling-rotation curves in the space of symmetric positive-definite matrices<sup>\*</sup>

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**Abstract:** We investigate a geometric structure on  $\text{Sym}^+(p)$ , the set of  $p \times p$  symmetric positive-definite (SPD) matrices, based on eigen-decomposition. Eigenstructure determines both a stratification of  $\text{Sym}^+(p)$ , defined by eigenvalue multiplicities, and fibers (preimages) of the “eigen-composition” map  $SO(p) \times \text{Diag}^+(p) \rightarrow \text{Sym}^+(p)$ . This leads to the notion of *scaling-rotation distance*, a measure of the minimal amount of scaling and rotation needed to transform an SPD matrix,  $X$ , into another,  $Y$ , by a smooth curve in  $\text{Sym}^+(p)$ . Our main goal in this paper is the systematic characterization and analysis of *minimal smooth scaling-rotation (MSSR) curves* [Jung et al. (2015)], images in  $\text{Sym}^+(p)$  of minimal-length geodesics connecting two fibers in the “upstairs” space  $SO(p) \times \text{Diag}^+(p)$ . The length of such a geodesic connecting the fibers over  $X$  and  $Y$  is exactly the scaling-rotation distance from  $X$  to  $Y$ . Characterizing MSSR curves raises basic questions: For which  $X, Y$  is there a *unique* MSSR curve from  $X$  to  $Y$ ? When there is more than one such curve, what is the set  $\mathcal{M}(X, Y)$  of MSSR curves from  $X$  to  $Y$ ? For  $p = 3$  we find new explicit formulas for MSSR curves and for the scaling-rotation distance, and identify  $\mathcal{M}(X, Y)$  in all “nontrivial” cases. For general  $p$  we translate uniqueness the questions into questions concerning distances between subspaces of  $\mathbf{R}^p$ , including some questions about the geometry of Grassmannians, and answer some of these questions.

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## 1. Introduction

In this work, we investigate a geometric structure on  $\text{Sym}^+(p)$ , the set of  $p \times p$  symmetric positive-definite (SPD) matrices, resulting from the stratification defined by eigenvalue multiplicities. This stratification is tied inextricably to our main goal in this paper: the systematic characterization and analysis of minimal smooth scaling-rotation curves. Such curves were defined in [14] as smooth curves whose length minimizes the amount of scaling and rotation needed to transform an SPD matrix into another. The techniques developed in this paper, when applied to the case  $p = 3$ , allow us to find new explicit formulas for such curves.

Recall that every  $X \in \text{Sym}^+(p)$  can be diagonalized by a rotation matrix:  $X = UDU^{-1} = UDU^T$  for some  $U \in SO(p), D \in \text{Diag}^+(p)$ . Here,  $\text{Diag}^+(p)$  denotes the set of  $p \times p$  diagonal matrices with positive entries. We refer to  $(U, D)$  as an *eigen-decomposition* of  $X$ . Conversely, for all  $U \in SO(p), D \in \text{Diag}^+(p)$ , the matrix  $UDU^T$  lies in  $\text{Sym}^+(p)$ . Thus the *space of eigen-decompositions* of  $p \times p$  SPD matrices is the manifold

$$M := M(p) := (SO \times \text{Diag})^+(p) := SO(p) \times \text{Diag}^+(p). \quad (1.1)$$

This manifold comes to us naturally equipped with a smooth surjective map  $F : M \rightarrow \text{Sym}^+(p)$  defined by

$$F(U, D) = UDU^T. \quad (1.2)$$

To define the set of eigen-decompositions corresponding to a single SPD matrix, for each  $X \in \text{Sym}^+(p)$ , we define the *fiber over  $X$*  to be the set

$$\mathcal{E}_X := F^{-1}(X) = \{(U, D) \in M : UDU^T = X\}$$

The relation  $\sim$  on  $M$  defined by lying in the same fiber—i.e.  $(U, D) \sim (V, \Lambda)$  if and only if  $F(U, D) = F(V, \Lambda)$ —is an equivalence relation. The quotient space  $M/\sim$  (the set of equivalence classes, endowed with the quotient topology) is canonically identified with  $\text{Sym}^+(p)$ . It should be noted that  $F$  is not a submersion (cf. [1, 5]), and that  $M$  is *not* a fiber bundle over  $\text{Sym}^+(p)$ ; as we will see explicitly later, the fibers are not all mutually diffeomorphic (or of the same dimension).

The different structures of fibers then naturally lead to a stratification of  $\text{Sym}^+(p)$  and  $M$ . The stratum to which an  $X \in \text{Sym}^+(p)$  belongs depends on the diffeomorphism type of  $\mathcal{E}_X$ . The stratification based on the fibers is equivalent to stratifications by orbit-type and eigenvalue-multiplicity type.

The strata of  $\text{Sym}^+(p)$  and  $M$  are determined by the patterns of eigenvalue multiplicities, and are labeled by partitions of the integer  $p$  and the set  $\{1, \dots, p\}$ . We will always assume  $p > 1$ , the case  $p = 1$  being uninteresting. For each  $p$ , one can obtain the numbers of strata (of  $\text{Sym}^+(p)$  and  $M$ ), the dimension of each stratum, and the diffeomorphism type of fibers belonging to each stratum. Several group-actions are involved, and the deepest understanding comes from identifying the relevant groups and the various actions.

In [16], Schwartzman introduced scaling-rotation curves as a way of interpolating between SPD matrices in such a way that eigenvectors and eigenvalues both change at uniform speed. To provide a geometric framework for these curves, Section 2 is devoted to systematic characterization of fibers and its connection to the stratification of  $\text{Sym}^+(p)$ . This allows to build upon the scaling-rotation framework for SPD matrices proposed in [14], which provides a geometric interpretation for the scaling-rotation curves in [16]. In particular, our characterization of fibers is essential in understanding differential topology and geometry of this framework.

In the scaling-rotation framework for SPD matrices, a distance  $d_{\mathcal{SR}}(X, Y)$  between any two matrices  $X, Y \in \text{Sym}^+(p)$  is measured by the minimal distance between fibers  $\mathcal{E}_X$  and  $\mathcal{E}_Y$ . For the distance between fibers in  $M$ , we choose the Riemannian structure on  $M = SO(p) \times \text{Diag}^+(p)$  as a product structure determined by bi-invariant Riemannian metrics  $g_{SO(p)}, g_{\mathcal{D}^+}$  on the two factors (each of which is a Lie group). The corresponding squared distance function  $d_M^2$  is a sum of squares. The geodesics connecting two fibers  $\mathcal{E}_X$  and  $\mathcal{E}_Y$  with the minimal length give rise to *minimal smooth scaling-rotation curves (MSSR) curves*, “efficient” scaling-rotation curves that join  $X$  and  $Y$ .

The geometry of  $SO(p) \times \text{Diag}^+(p)$  with the metric  $d_M$  is relatively simple. Despite this simplicity “upstairs”, the problem of determining MSSR curves between arbitrary  $X, Y$  in the quotient space  $\text{Sym}^+(p)$  is far from trivial, and the dependence on  $X$  and  $Y$  of the set  $\mathcal{M}(X, Y)$  of such curves is surprisingly intricate. While it is easy to write down an explicit formula for the distance between two arbitrary *points* of  $SO(p) \times \text{Diag}^+(p)$ , even in Euclidean space there is no formula for distance between submanifolds of positive dimension, even when the submanifolds come equipped with explicit parametrizations or are level-sets of explicitly given functions. The MSSR curves are images of shortest-length geodesics between two submanifolds  $\mathcal{E}_X$  and  $\mathcal{E}_Y$ . These shortest-length geodesics are not unique, and their characterization depends on the diffeomorphism types of  $X$  and  $Y$ . For some pairs  $(X, Y)$ , these minimal geodesics all correspond to a unique MSSR curve ( $|\mathcal{M}(X, Y)| = 1$ ); for other pairs  $(X, Y)$ , they provide multiple MSSR curves ( $|\mathcal{M}(X, Y)| > 1$ ).

To have  $|\mathcal{M}(X, Y)| > 1$  there must be distinct shortest-length geodesics  $\gamma_1, \gamma_2 : [0, 1] \rightarrow (SO \times \text{Diag}^+(p))$  from  $\mathcal{E}_X \rightarrow \mathcal{E}_Y$  such that  $F \circ \gamma_1 \neq F \circ \gamma_2$ . There are essentially two ways, not mutually exclusive, that this non-uniqueness can arise: (i) there exist such  $\gamma_i$  ( $i = 1, 2$ ) with distinct endpoint-pairs  $((\gamma_1(0), \gamma_1(1)) \neq (\gamma_2(0), \gamma_2(1)))$ , and (ii) there exist such  $\gamma_i$  with identical endpoint-pairs  $((\gamma_1(0), \gamma_1(1)) = (\gamma_2(0), \gamma_2(1)))$ . We call these possibilities “Type I” and “Type II” non-uniqueness, respectively. Surprisingly, the seemingly *ad hoc* question of whether Type II non-uniqueness occurs is closely related to a question purely about the geometry of Grassmannians equipped with a standard Riemannian metric: for  $m$  even and positive, is every  $m$ -dimensional subspace of  $\mathbf{R}^p$  within a certain distance  $c(m)$  of a coordinate  $m$ -plane? We obtain the Type-II-nonuniqueness results above by showing that for  $p \leq 4$  (respectively,  $p \geq 11$ ), the answer to the latter question is yes (respectively, no) for the case  $m = 2$ , and by showing that these answers imply our results. Although our

interest in the question concerning the geometry of Grassmannians was originally motivated by our interest in MSSR curves, our study of this question may be of independent interest, as may be our investigation of certain related questions concerning distances between even-dimensional subspaces of  $\mathbf{R}^p$  and even-dimensional coordinate planes not necessarily of the same dimension.

Understanding the stratification enables us to analyze some non-trivial features of the scaling-rotation framework. For example,  $d_{\mathcal{SR}}$  is a metric on the top stratum of  $\text{Sym}^+(p)$ , but is not a metric on all of  $\text{Sym}^+(p)$ . For any  $p$ , the analysis of  $d_{\mathcal{SR}}(X, Y)$  and MSSR curves depend on the strata to which  $X$  and  $Y$  belong, because fibers are topologically and geometrically different for different strata. As noted above, MSSR curves from  $X$  to  $Y$  whose lengths equal  $d_{\mathcal{SR}}(X, Y)$  are not always unique. For  $p = 3$ , quaternionic methods enable us to provide closed-form formulas for  $d_{\mathcal{SR}}(X, Y)$  for all non-trivial cases. In addition, for those cases, we explicitly describe the set of MSSR curves from  $X$  to  $Y$ .

Our study of the stratification of  $\text{Sym}^+(p)$  is motivated in part by the special case of  $3 \times 3$  SPD matrices. In particular, in diffusion tensor imaging (DTI), a diffusion tensor is viewed as an ellipsoid, represented by a  $3 \times 3$  SPD matrix. DTI researchers are interested in the classification of ‘noisy’ tensors into strata [20]. Our eigenvalue-multiplicity stratification categorizes the ellipsoids associated with the SPD matrices into distinct shapes, which in the case  $p = 3$  are known as spherical, prolate/oblate, and tri-axial (scalene).

In recent years there has been increased interest in stratified manifolds for statistical applications. For example, stratified manifolds have recently received attention in the study of phylogenetic trees [4, 13] and Kendall’s 3D shape space [15]. New analytic tools for such manifolds are fast developing [6, 2]. Our work contributes to the development of such tools on both a theoretical and practical level, providing a solid geometrical foundation for development of statistical procedures on the stratified manifold  $\text{Sym}^+(p)$ .

The rest of this paper is organized as follows. In Section 2 we identify all the fibers of the eigen-composition map  $F$  systematically in terms of partitions of the integer  $p$  and the set  $\{1, 2, \dots, p\}$ . This culminates in Section 2.5 with a very explicit description of all the fibers. In Section 3 we show how these ideas lead to stratifications of  $\text{Sym}^+(p)$ ; we provide some examples for  $p = 2$  and  $p = 3$  in Section 3.3. In Section 4 we discuss the geometry of scaling-rotation framework. This includes subsection 4.3 on uniqueness questions for MSSR curves. The mathematical analysis of these questions entails a significant digression from the main track of the paper, so most of this analysis (and the proofs of most results stated in Section 4.3) is deferred to the Appendix. Closed-form expressions for the scaling-rotation distance and a catalog of the “nontrivial” unique and non-unique cases of MSSR curves for the important  $p = 3$  case are given in Sections 5 and 6. Some pictorial examples of these MSSR curves (including cases omitted from the catalog in Section 6) are contained in the online supplement. The online supplement also contains examples for the case  $p = 2$ . The Appendix (Section 7) provides the proofs of results in Section 4.3. This is achieved by translating the questions in Section 4.3 into questions concerning distances between subspaces of  $\mathbf{R}^p$ , including some questions about the geometry of Grassmannians. As noted

earlier, some of the results in the Appendix may thus be of interest outside the scope of this paper.

In this paper, we will encounter numerous instances of a group  $G$  acting from the left on a space  $X$ . We will use the notation  $(g, x) \mapsto g \cdot x$  for all such actions (where  $g \in G, x \in X$ ), and  $X/G$  will always denote the corresponding quotient space (the space of orbits, with the quotient topology). When  $X$  is a finite set, we always give  $X$  (and therefore  $X/G$ ) the discrete topology.

## 2. Partitions and Fibers

### 2.1. Partitions of $p$ and $\{1, 2, \dots, p\}$

We will consider several stratified spaces in this paper. The strata we define will be labeled by two different types of *partitions*. For the sake of efficiency we first review these partitions and fix some related notation.

Recall that a partition of the *positive integer*  $p$  is a (necessarily finite) sequence of positive integers  $k_1 \geq k_2 \geq k_3 \geq \dots$  with  $\sum k_i = p$ , while a partition of the *set*  $\{1, 2, \dots, p\}$  is a (necessarily finite) collection  $J = \{J_1, J_2, \dots\}$  of one or more nonempty, pairwise disjoint subsets  $J_i$  whose union is  $\{1, 2, \dots, p\}$ . Partitions of an integer are commonly written using additive notation, e.g.  $2 + 2 + 1$  instead of  $2, 2, 1$  (a partition of 5). In a partition  $k_1, k_2, \dots$  of  $p$ , the terms  $k_i$  of the sequence are called the *parts* of the partition (and are counted with multiplicity; the parts of  $2 + 2 + 1$  are 2, 2, and 1). For a partition of  $p$  with  $r$  parts, we will also use the ordered  $r$ -tuple  $(k_1, \dots, k_r)$  or multi-set notation  $\{k_1, \dots, k_r\}$  to denote the partition  $k_1, \dots, k_r$ . In a partition  $J = \{J_1, J_2, \dots\}$ , the  $J_i$  are called the *blocks* of  $J$ .

**Remark 2.1** While we have used the most common definition of “partition of  $p$ ”, a definition more directly suited to our needs comes from considering *ordered* and *unordered partitions*. An *ordered partition* of  $p$  is a sequence of positive integers  $k_1, k_2, \dots$  with  $\sum_i k_i = p$ . We call two ordered partitions of  $p$  *equivalent* if one is a re-ordering of the other; this is obviously an equivalence relation on the set of ordered partitions. An *unordered partition* of  $p$  is an equivalence class under this relation. Since each equivalence class contains a “standard representative”, the unique representative in which the sequence  $k_1, k_2, \dots$  is non-increasing, there is a natural one-to-one correspondence between *unordered partitions of  $p$*  and *partitions of  $p$* , so we could just as well take the definition of “partition of  $p$ ” to be “unordered partition of  $p$ ”. We have used the common definition of “partition of  $p$ ” to avoid extra notational baggage. However, for our purposes, it is best to regard a partition of  $p$  as intrinsically being an *unordered* object that, for notational simplicity only, we are writing down in a standardized way that happens to make it appear ordered.

### Notation 2.2

1. We write  $\text{Part}(\{1, \dots, p\})$  for the set of partitions of  $\{1, 2, \dots, p\}$ , and  $\text{Part}(p)$  for the set of partitions of  $p$ .

Partitions of $\{1, 2, 3\}$		Partitions of 3	
$J_{\text{top}} = \{\{1\}, \{2\}, \{3\}\}$	$J_{\text{top}}$	$\mapsto$	$[J_{\text{top}}] = 1 + 1 + 1$
$J_3 = \{\{1, 2\}, \{3\}\}$	$\swarrow \downarrow \searrow$		$\downarrow$
$J_2 = \{\{1, 3\}, \{2\}\}$	$J_1 \quad J_2 \quad J_3$	$\mapsto$	$[J_1] = [J_2] = [J_3] = 2 + 1$
$J_1 = \{\{2, 3\}, \{1\}\}$	$\searrow \downarrow \swarrow$		$\downarrow$
$J_{\text{bot}} = \{\{1, 2, 3\}\}$	$J_{\text{bot}}$	$\mapsto$	$[J_{\text{bot}}] = 3$

TABLE 1

Part( $\{1, 2, 3\}$ ) and Part(3). The relation  $J_2 \leftarrow J_{\text{top}}$  stands for  $J_2 \leq J_{\text{top}}$  (i.e.,  $J_{\text{top}}$  refines  $J_2$ ). None of  $J_1, J_2, J_3$ , refines either of the others.  $[J_{\text{top}}]$  refines  $[J_2]$ .

2. The natural left-action of the symmetric group  $S_p$  on  $\{1, 2, \dots, p\}$  induces left-actions of  $S_p$  on  $\text{Part}(\{1, \dots, p\})$  and  $\mathbf{R}^p$ , given by

$$\pi \cdot \{J_1, J_2, \dots, J_r\} = \{\pi(J_1), \pi(J_2), \dots, \pi(J_r)\}, \quad (2.1)$$

$$\pi \cdot (x_1, x_2, \dots, x_p) = (x_{\pi^{-1}(1)}, x_{\pi^{-1}(2)}, \dots, x_{\pi^{-1}(p)}), \quad (2.2)$$

where  $\pi \in S_p$  and  $J \in \text{Part}(\{1, \dots, p\})$ . For  $J \in \text{Part}(\{1, \dots, p\})$ , we write  $[J]$  for its image in the quotient space  $\text{Part}(\{1, \dots, p\})/S_p$ .

There is an obvious  $S_p$ -invariant map  $\text{Part}(\{1, \dots, p\}) \rightarrow \text{Part}(p)$  that assigns to  $J = \{J_1, \dots, J_r\}$  the sequence  $|J_1|, \dots, |J_r|$ , rearranged in nonincreasing order. This map induces a bijection  $\text{Part}(\{1, \dots, p\})/S_p \rightarrow \text{Part}(p)$ . *Henceforth we will use this bijection implicitly and will regard  $\text{Part}(\{1, \dots, p\})/S_p$  and  $\text{Part}(p)$  as the same set*; e.g. we will generally write  $[J]$  for a typical element of  $\text{Part}(p)$ .

The sets  $\text{Part}(\{1, \dots, p\})$  and  $\text{Part}(p)$  are partially ordered by the *refinement* relation. For  $J, K \in \text{Part}(\{1, \dots, p\})$ , we say that  $K$  is a *refinement* of  $J$ , or that  $K$  *refines*  $J$ , if every element of  $K$  is a subset of an element of  $J$  (remember that an *element* of  $K$  or  $J$  is a *subset* of  $\{1, \dots, p\}$ ); equivalently, if  $K$  can be obtained by partitioning the elements of  $J$ . We write  $J \leq K$  if  $K$  refines  $J$ ; “ $\leq$ ” is then a partial ordering on  $\text{Part}(\{1, \dots, p\})$ . (The reason we write  $J \leq K$  rather than the “ $K \leq J$ ” one might expect for this refinement-relation will be clear later.) Similarly, for  $[J], [K] \in \text{Part}(p)$ , we say that  $[K]$  is a *refinement* of  $[J]$ , or that  $[K]$  *refines*  $[J]$ , if  $[K]$  can be obtained by partitioning the parts of  $[J]$ . (For example,  $\{3, 2, 2\}$  refines  $\{7\}$ ,  $\{5, 2\}$ , and  $\{4, 3\}$ , but neither of  $\{3, 3, 2\}$ ,  $\{4, 1, 1, 1\}$  refines the other.) We write  $[J] \leq [K]$  if  $[K]$  refines  $[J]$ ; this “ $\leq$ ” is a partial ordering on  $\text{Part}(p)$ . Note that the quotient map  $\text{Part}(\{1, \dots, p\}) \rightarrow \text{Part}(\{1, \dots, p\})/S_p = \text{Part}(p)$  is order-preserving. These relations are illustrated for  $p = 3$  in Table 1.

For all partial-order relations “ $\leq$ ” in this paper, the meanings of the symbols “ $<$ ”, “ $\geq$ ”, and “ $>$ ” are defined from “ $\leq$ ” the obvious way. Note that there is a well-defined largest (also called highest) and smallest (also called lowest) element of  $\text{Part}(\{1, \dots, p\})$  and of  $\text{Part}(p)$ : for all  $J \in \text{Part}(\{1, \dots, p\})$ , we have

$$J_{\text{bot}} := \{\{1, 2, \dots, p\}\} \leq J \leq \{\{1\}, \{2\}, \dots, \{p\}\} =: J_{\text{top}},$$

$$\{p\} \leq [J] \leq \{1, 1, \dots, 1\}.$$

We always assume  $p > 1$ , so  $J_{\text{top}} \neq J_{\text{bot}}$ .

## 2.2. Relation of partitions to eigenstructure

**Definition 2.3** Let  $\text{Diag}(p)$  denote the set of  $p \times p$  diagonal matrices, and let  $\text{Diag}^+(p) := \{\text{diag}(d_1, \dots, d_p) : d_i > 0, 1 \leq i \leq p\} \subset \text{Diag}(p)$ . For  $D = \text{diag}(d_1, \dots, d_p) \in \text{Diag}(p)$ , let  $J_D$  denote the partition of  $\{1, 2, \dots, p\}$  determined by the equivalence relation  $i \sim_D j \iff d_i = d_j$ .

Various objects we can define that depend on  $D$  actually depend only on the partition  $J_D$ . As  $D$  runs over all of  $\text{Diag}^+(p)$ , the partitions  $J$  run over all of  $\text{Part}(\{1, \dots, p\})$ . For this reason we define certain objects, such as the groups  $G_J$  below, in terms of general partitions  $J$  of  $\text{Part}(\{1, \dots, p\})$ .

**Definition 2.4** For  $\emptyset \neq J \subset \{1, 2, \dots, p\}$ , let  $\mathbf{R}^J \subset \mathbf{R}^p$  denote the subspace  $\{(x_1, \dots, x_p) \in \mathbf{R}^p \mid x_j = 0 \ \forall j \notin J\}$ . For a partition  $J = \{J_1, \dots, J_r\}$  of  $\{1, 2, \dots, p\}$ , let  $\{W_1, \dots, W_r\} = \{W_1^J, \dots, W_r^J\} = \{\mathbf{R}^{J_1}, \dots, \mathbf{R}^{J_r}\}$  denote the corresponding subspaces of  $\mathbf{R}^p$ ; note that we have an orthogonal decomposition  $\mathbf{R}^p = \mathbf{R}^{J_1} \oplus \dots \oplus \mathbf{R}^{J_r}$ . Define the subgroup  $G_J \subset SO(p)$  by

$$G_J = \{R \in SO(p) \mid RW_i = W_i, 1 \leq i \leq r\}, \quad (2.3)$$

a Lie group with (generally) more than one connected component. We write  $G_J^0$  for the identity component of  $G_J$  (the connected component of  $G_J$  containing the identity).

If each block  $J_i$  consists of consecutive integers, then the elements of  $G_J$  are block-diagonal. For example, if  $p = 5$  and  $J = \{\{1, 2\}, \{3, 4, 5\}\}$ , then

$$\begin{aligned} G_J &= \left\{ \begin{bmatrix} R_1 & 0 \\ 0 & R_2 \end{bmatrix} : R_1 \in O(2), R_2 \in O(3), \det(R_1)\det(R_2) = 1 \right\} \\ &\cong S(O(2) \times O(3)). \end{aligned}$$

In this example,  $G_J$  has two connected components, one in which  $\det(R_1) = \det(R_2) = 1$  (the component  $G_J^0$ ), and one in which  $\det(R_1) = \det(R_2) = -1$ .

For general  $J$ , the elements of  $G_J$  have “interleaved blocks”. With notation as in Definition 2.4, note that

$$G_J \cong S(O(W_1) \times O(W_2) \times \dots \times O(W_r)) \quad (2.4)$$

$$\cong S(O(|J_1|) \times O(|J_2|) \cdots \times O(|J_r|)). \quad (2.5)$$

(Here  $O(W_i)$  denotes the orthogonal group of the subspace  $W_i$ , which we identify with a subgroup of  $O(p)$ . For any subgroup  $H \subset O(p)$ , we write  $S(H)$  for  $H \cap SO(p)$ .) The identity component  $G_J^0$  is isomorphic to  $SO(W_1) \times SO(W_2) \times \dots \times SO(W_r)$ . Hence, writing  $k_i = |J_i|$ , we have

$$G_J^0 \cong SO(k_1) \times SO(k_2) \cdots \times SO(k_r). \quad (2.6)$$

Obviously (2.4) holds whether or not  $k_1 \geq k_2 \geq \dots \geq k_r$ . However, if the  $k_i$  are non-decreasing then  $[J] = (k_1, \dots, k_r)$ , so for the sake of concreteness we define

$$G_{[J]}^0 = SO(k_1) \times SO(k_2) \cdots \times SO(k_r) \quad \text{if } [J] = (k_1, k_2, \dots, k_r).$$

**Remark 2.5** A easily-verified feature that the groups  $G_J$  have that is reflected in the stratifications of  $\text{Sym}^+(p)$  and  $M$  discussed in Section 3 is the following:

$$J \leq K \iff G_J \supset G_K. \quad (2.7)$$

To relate the groups  $G_J$  to eigenstructure, for each  $D \in \text{Diag}(p)$  let

$$G_D = \{R \in SO(p) : RD = DR\} = \{R \in SO(p) : RDR^{-1} = D\}, \quad (2.8)$$

the *stabilizer of  $D$*  under the action of  $SO(p)$  on  $\text{Sym}(p)$  by conjugation, and observe that if  $(U, D) \in M$  is an eigen-decomposition of  $X \in \text{Sym}^+(p)$ , and  $R$  lies in  $G_D$ , then  $(UR, D)$  is also an eigen-decomposition of  $X$ . But  $G_D$  is precisely the group  $G_{J_D}$  defined using Definitions 2.3 and 2.4. (In other words, the group  $G_D$  does not depend on the absolute or relative sizes of the diagonal entries of  $D$ , but only on which eigenvalues are equal to which other eigenvalues.)

### 2.3. A non-split extension of the symmetric group

In this subsection we define two groups,  $\tilde{S}_p$  and  $\tilde{S}_p^+$ , the second a subgroup of the first. Both extend the symmetric group  $S_p$ , but  $\tilde{S}_p$  is a split extension (a semidirect product) while  $\tilde{S}_p^+$  is not. In the next subsection we interpret these groups in terms of matrices; however, viewing these groups purely as matrix groups can obscure some of the structure of the fibers of  $F$ .

#### Notation 2.6

1. We write  $\mathcal{I}_p$  for the group  $(\mathbf{Z}_2)^p = \mathbf{Z}_2 \times \mathbf{Z}_2 \times \cdots \times \mathbf{Z}_2$ . The role of  $\mathbf{Z}_2$  will be as the *group of signs*, so we write it multiplicatively, with elements  $\pm 1$ . We will write typical elements of  $\mathcal{I}_p$  as  $\sigma = (\sigma_1, \dots, \sigma_p)$ . We call  $\mathcal{I}_p$  the *group of sign-changes*, and write  $\mathbf{1}$  for its identity element.

2. For  $\pi \in S_p$ ,  $\sigma = (\sigma_1, \dots, \sigma_p) \in \mathcal{I}_p$ , in accordance with (2.2) we set

$$\pi \cdot \sigma = (\sigma_{\pi^{-1}(1)}, \dots, \sigma_{\pi^{-1}(p)}). \quad (2.9)$$

**Definition 2.7** The *sign homomorphism*  $\text{sgn} : \mathcal{I}_p \rightarrow \mathbf{Z}_2$  is the map defined by

$$\text{sgn}(\sigma_1, \dots, \sigma_p) = \prod_{i=1}^p \sigma_i. \quad (2.10)$$

Observe that  $\text{sgn} : \mathcal{I}_p \rightarrow \mathbf{Z}_2$  is indeed a homomorphism, and is  $S_p$ -invariant:

$$\text{sgn}(\pi \cdot \sigma) = \text{sgn}(\sigma) \text{ for all } \pi \in S_p, \sigma \in \mathcal{I}_p. \quad (2.11)$$

We also write “sgn” for the usual sign-homomorphism  $S_p \rightarrow \mathbf{Z}_2$ . Both of these sign-homomorphisms determine index-two subgroups, the sets of elements of sign 1. For  $\mathcal{I}_p$ , our notation for this subgroup will be

$$\mathcal{I}_p^+ := \{\sigma \in \mathcal{I}_p : \text{sgn}(\sigma) = 1\}$$



For  $S_p$ , of course, the corresponding subgroup is the group of even permutations (the *alternating group*  $A_p$ ). By analogy, we call  $\mathcal{I}_p^+$  the group of *even sign-changes*.

One may easily check that (2.9) defines a left action of the symmetric group on  $\mathcal{I}_p$ , and that “ $\pi \cdot$ ” :  $\mathcal{I}_p \rightarrow \mathcal{I}_p$  is an automorphism. Hence this action determines a *semidirect product* group: a group

$$\tilde{S}_p = \mathcal{I}_p \rtimes S_p \quad (2.12)$$

whose underlying set is  $\mathcal{I}_p \times S_p$ , and which contains subgroups  $\mathcal{I}_p \times \{\text{id.}\}$  and  $\{\mathbf{1}\} \times S_p$  isomorphic to  $\mathcal{I}_p, S_p$ , respectively, but in which the group operation is given by

$$(\sigma_1, \pi_1)(\sigma_2, \pi_2) = (\sigma_1(\pi_1 \cdot \sigma_2), \pi_1 \pi_2). \quad (2.13)$$

Thus  $\tilde{S}_p$  is a *split extension* of the symmetric group: the short exact sequence

$$1 \rightarrow \mathcal{I}_p \xrightarrow{\text{incl}} \tilde{S}_p \xrightarrow{\text{proj}_2} S_p \rightarrow 1 \quad (2.14)$$

is split by the homomorphism  $S_p \rightarrow \tilde{S}_p$  given by  $\pi \mapsto (\mathbf{1}, \pi)$ . (Here “incl” is the map  $\sigma \mapsto (\sigma, \text{id.})$ , and  $\text{proj}_2$  is the projection map  $(\sigma, \pi) \mapsto \pi$ .)

Because of (2.11), the sign-homomorphisms  $\mathcal{I}_p \rightarrow \mathbf{Z}_2, S_p \rightarrow \mathbf{Z}_2$  determine a third sign-homomorphism  $\text{sgn} : \tilde{S}_p \rightarrow \mathbf{Z}_2$ , defined by

$$\text{sgn}(\sigma, \pi) = \text{sgn}(\sigma) \text{sgn}(\pi). \quad (2.15)$$

**Definition 2.8** We write  $\tilde{S}_p^+$  for  $\ker(\text{sgn} : \tilde{S}_p \rightarrow \mathbf{Z}_2)$ , an index-two subgroup of  $\tilde{S}_p$ . Equivalently,  $\tilde{S}_p^+ = \{(\sigma, \pi) \in \tilde{S}_p : \text{sgn}(\sigma) = \text{sgn}(\pi)\}$ .

The group  $\tilde{S}_p^+$  is another extension of the symmetric group; we have a short exact sequence

$$1 \rightarrow \mathcal{I}_p^+ \xrightarrow{\text{incl}} \tilde{S}_p^+ \xrightarrow{\text{proj}_2} S_p \rightarrow 1. \quad (2.16)$$

However,  $\tilde{S}_p^+$  is a *non-split* extension of  $S_p$ ; there is *no* homomorphism  $\beta : S_p \rightarrow \tilde{S}_p^+$  such that  $\text{proj} \circ \beta = \text{identity map}$ . (We leave the proof of this fact to the interested reader. The fact that (2.16) does not split is motivational—it is an obstruction to doing certain constructions in an algebraically simpler way—but is not something upon which any of our results rely.)

**Remark 2.9** It is easily seen that  $\mathcal{I}_p^+$  is isomorphic to  $(\mathbf{Z}_2)^{p-1}$ , though not canonically. (For example, one isomorphism  $(\mathbf{Z}_2)^{p-1} \rightarrow \mathcal{I}_p^+$  is  $(\sigma_1, \dots, \sigma_{p-1}) \mapsto (\sigma_1, \dots, \sigma_{p-1}, \prod_{i=1}^{p-1} \sigma_i)$ . Thus the short exact sequences (2.14) and (2.16) can alternatively be written as

$$1 \rightarrow (\mathbf{Z}_2)^p \rightarrow \tilde{S}_p \rightarrow S_p \rightarrow 1 \quad (2.17)$$

and

$$1 \rightarrow (\mathbf{Z}_2)^{p-1} \rightarrow \tilde{S}_p^+ \rightarrow S_p \rightarrow 1. \quad (2.18)$$

**Result 2.10** *The orders (cardinalities) of the groups  $\tilde{S}_p$  and  $\tilde{S}_p^+$  are as follows:*

$$|\tilde{S}_p| = 2^p p! , \quad |\tilde{S}_p^+| = 2^{p-1} p! . \quad (2.19)$$

**Proof:** These formulas follow immediately from (2.12) and the fact that  $\tilde{S}_p^+$  has index 2 in  $\tilde{S}_p$ . (They also follow immediately from (2.17)–(2.18).) ■

**Remark 2.11** For a subspace  $W \subset \mathbf{R}^p$  and  $\epsilon \in \mathbf{Z}_2 = \{\pm 1\}$ , let  $O_\epsilon(W) \subset O(W)$  denote the set of orthogonal transformations with determinant  $\epsilon$ . In the setting of (2.4), the connected components of  $G_J$  are  $O_{\epsilon_1}(W_1) \times O_{\epsilon_2}(W_2) \times \cdots \times O_{\epsilon_r}(W_r)$ , subject to the restriction  $\prod_i \epsilon_i = 1$ . Thus a labeling of the blocks of an  $r$ -block partition  $J$  yields a 1-1 correspondence between  $\mathcal{I}_r^+$  and the set of connected components of  $G_J$ . In particular, the number of connected components is  $2^{r-1}$ .

#### 2.4. Signed permutation matrices

The group  $\tilde{S}_p$  has a natural representation on  $\mathbf{R}^p$ , the map  $\mathbf{mat} : \tilde{S}_p \rightarrow O(p)$  defined by

$$\mathbf{mat}(\sigma, \pi) = I_\sigma P_\pi , \quad (2.20)$$

where  $I_\sigma = \text{diag}(\sigma_1, \dots, \sigma_p)$  and  $P_\pi$  is the matrix of the linear map “ $\pi \cdot$ ” :  $\mathbf{R}^p \rightarrow \mathbf{R}^p$  in (2.2). The entries of the permutation matrix  $P_\pi$  are  $(P_\pi)_{ij} = \delta_{i, \pi(j)}$ . (We will see shortly that  $\mathbf{mat}$  is a homomorphism, justifying the term “representation on  $\mathbf{R}^p$ ”.) It is easily seen that  $\mathbf{mat}$  is injective.

**Definition 2.12** We call a  $p \times p$  matrix  $P$  a *signed permutation matrix* if for some (necessarily unique)  $\pi \in S_p$  the entries of  $P$  satisfy  $P_{ij} = \pm \delta_{i, \pi(j)}$ . We call such  $P$  *even* if  $\det(P) = 1$  and *odd* if  $\det(P) = -1$ . (Note that evenness of  $P$  is not the same as evenness of the associated permutation  $\pi$ .) The set of signed  $p \times p$  permutation matrices is exactly  $\mathbf{mat}(\tilde{S}_p) \subset O(p)$ ; the subset of even elements is exactly  $\mathbf{mat}(\tilde{S}_p^+) \subset SO(p)$ .

It is easy to see that  $\mathbf{mat}(\tilde{S}_p)$  is actually a subgroup of  $O(p)$ . (This also follows from the fact, shown below, that  $\mathbf{mat}$  is a homomorphism  $\tilde{S}_p \rightarrow O(p)$ .) Furthermore, at the level of matrices, the sign-homomorphism  $\tilde{S}_p \rightarrow \mathbf{Z}_2$  is simply determinant:

$$\text{sgn}(\sigma, \pi) = \det(\mathbf{mat}(\sigma, \pi)) = \det(I_\sigma P_\pi). \quad (2.21)$$

It follows that  $\mathbf{mat}(\tilde{S}_p^+)$  is a subgroup of  $SO(p)$ .

Identifying  $\text{Diag}^+(p)$  with  $(\mathbf{R}_+)^p \subset \mathbf{R}^p$ , the action (2.2) yields an action of  $S_p$  on  $\text{Diag}^+(p)$ , given by

$$\begin{aligned} \pi \cdot \text{diag}(\mathbf{d}) &= \text{diag}(\pi \cdot \mathbf{d}) \\ &= \text{diag}(d_{\pi^{-1}(1)}, \dots, d_{\pi^{-1}(p)}) \quad \text{if } \mathbf{d} = (d_1, \dots, d_p). \end{aligned} \quad (2.22)$$

**Notation 2.13** For  $D \in \text{Diag}^+(p)$ , we write  $[D]$  for its image in the quotient space  $\text{Diag}^+(p)/S_p$ .

One may easily check that for any  $\pi \in S_p$ ,  $D \in \text{Diag}(p)$ , we have

$$\pi \cdot D = P_\pi D (P_\pi)^T = P_\pi D (P_\pi)^{-1}, \quad (2.23)$$

and that the restrictions of the map  $\text{mat}$  to the subgroups  $\mathcal{I}_p \times \{\text{id.}\} \cong \mathcal{I}_p$  and  $\{\mathbf{1}\} \times S_p \cong S_p$  are homomorphisms. It follows easily that the map  $\text{mat} : \tilde{S}_p \rightarrow O(p) \subset GL(p, \mathbf{R})$  is a homomorphism (hence a representation on  $\mathbf{R}^p$ , as asserted earlier):

$$\begin{aligned} \text{mat}(\sigma_1, \pi_1) \text{mat}(\sigma_2, \pi_2) &= I_{\sigma_1} P_{\pi_1} I_{\sigma_2} (P_{\pi_1})^{-1} P_{\pi_1} P_{\pi_2} \\ &= I_{\sigma_1} (\pi_1 \cdot I_{\sigma_2}) P_{\pi_1 \pi_2} \\ &= I_{\sigma_1} I_{\pi_1 \cdot \sigma_2} P_{\pi_1 \pi_2} \\ &= I_{\sigma_1 (\pi_1 \cdot \sigma_2)} P_{\pi_1 \pi_2} \\ &= \text{mat}((\sigma_1, \pi_1)(\sigma_2, \pi_2)). \end{aligned}$$

Since  $\text{mat}$  is an injective homomorphism, it is an isomorphism onto its image, the subgroup  $\text{mat}(\tilde{S}_p) \subset O(p)$ .

A copy of the symmetric group sits as  $\text{mat}(S_p) \subset \text{mat}(\tilde{S}_p)$ . The non-splitting of the exact sequence (2.16) is equivalent to the fact that there exists no sgn-preserving map  $\text{mat}(S_p) \rightarrow \mathcal{I}_p$ ,  $\pi \mapsto \sigma_\pi$ , such that the map  $\pi \mapsto I_{\sigma_\pi} P_\pi$  has image in  $\text{mat}(\tilde{S}_p^+)$  and is a homomorphism. (We leave this non-existence proof to the interested reader as well; again, this non-existence motivates some of our methods, but nothing that we do assumes it.)

As in [14], we call the elements of  $\text{mat}(\mathcal{I}_p)$  *sign-change matrices*, even or odd according to their determinants.

For any subgroup  $H$  of  $\tilde{S}_p$ ,  $\text{mat}$  restricts to an isomorphism  $H \rightarrow \text{mat}(H)$ . Therefore to simplify notation, *henceforth in most expressions we will not write the map  $\text{mat}$  explicitly*; rather, we will use (for example) the notation  $\tilde{S}_p$  for both  $\tilde{S}_p$  and  $\text{mat}(\tilde{S}_p)$ . It should always be clear from context whether our notation refers to an element (or subgroup) of  $\tilde{S}_p$ , or the corresponding matrix (or finite group of matrices) under the map  $\text{mat}$ . However, to avoid some odd-looking formulas we will use the following notation:

**Notation 2.14** We write typical elements of the (abstract) signed-permutation group  $\tilde{S}_p$  as  $g$ , and define the matrix  $P_g = \text{mat}(g) \in \tilde{S}_p$ . Thus  $P_{(\sigma, \pi)} = I_\sigma P_\pi$ . The image of  $g$  under the projection  $\text{proj}_2 : \tilde{S}_p \rightarrow S_p$  will be denoted  $\pi_g$ .

We remark that if  $\tilde{S}_p$  is interpreted as  $\text{mat}(\tilde{S}_p)$ ,  $\text{proj}_2$  is the map  $\mathcal{I}_\sigma P_\pi \mapsto \pi$  (well-defined, since every element of  $\text{mat}(\tilde{S}_p)$  can be written *uniquely* in the form  $\mathcal{I}_\sigma P_\pi$ ).

Note that the action of  $S_p$  on  $\text{Diag}^+(p)$  lifts to an action of  $\tilde{S}_p$  on  $\text{Diag}^+(p)$ :

$$g \cdot D := \pi_g \cdot D. \quad (2.24)$$

In terms of matrices, this is just the conjugation action:

$$P_{(\sigma, \pi)} \cdot D = I_\sigma P_\pi D P_\pi^{-1} I_\sigma^{-1} = P_\pi D P_\pi^{-1}, \quad (2.25)$$

the latter equality holding since sign-change matrices are diagonal (and therefore commute with diagonal matrices).

We end this (sub-)subsection with an easy lemma that will be used in the proof of Proposition 2.16 in the next (sub-)subsection:

**Lemma 2.15**  $\mathcal{I}_p^+ \subset G_J$  for all  $J \in \text{Part}(\{1, \dots, p\})$ .

**Proof:** Here  $\mathcal{I}_p^+$  literally means  $\text{mat}(\mathcal{I}_p^+)$ , of course, which is the same set as  $\text{Diag}(p) \cap SO(p)$ . Since for any invertible diagonal matrix  $L$  and any nonempty  $J \subset \{1, \dots, p\}$  we have  $L\mathbf{R}^J = \mathbf{R}^J$ , it follows from (2.3) that  $\text{Diag}(p) \cap SO(p) \subset G_J$  for all  $J \in \text{Part}(\{1, \dots, p\})$ . ■

### 2.5. Structure of the fibers

In this subsection we will provide a systematic description of the fibers of  $F$ . The starting point is the following proposition, a corollary of [14, Theorem 3.3].

**Proposition 2.16** Let  $X \in \text{Sym}^+(p)$ ,  $(U, D) \in \mathcal{E}_X = F^{-1}(X)$ . Then

$$\mathcal{E}_X = \{(URP^{-1}, PDP^{-1}) : R \in G_D, P \in \text{mat}(\tilde{S}_p^+)\}. \quad (2.26)$$

**Proof:** Equation (2.26) can be rewritten as

$$\mathcal{E}_X = \{(U(P_g R)^{-1}, \pi_g \cdot D) : R \in G_D, g \in \tilde{S}_p^+\}. \quad (2.27)$$

Let  $\sigma_1 = (-1, 1, 1, \dots, 1)$  (with a 1 in every entry but the first). Define functions  $s_1 : S_p \rightarrow \mathcal{I}_p$  and  $s : S_p \rightarrow \tilde{S}_p^+$  by

$$s_1(\pi) = \begin{cases} \mathbf{1} & \text{if } \pi \text{ is even,} \\ \sigma_1 & \text{if } \pi \text{ is odd,} \end{cases} \quad (2.28)$$

$$s(\pi) = (s_1(\pi), \pi). \quad (2.29)$$

Thus  $P_{s(\pi)} = I_{s_1(\pi)} P_\pi$ . The map  $s$  is *not* a homomorphism, but *is* a right-inverse of  $\text{proj}_2 : \tilde{S}_p^+ \rightarrow S_p$ , one of many systematic but otherwise arbitrary choices among all right-inverses of  $\text{proj}_2|_{\tilde{S}_p^+}$ . (None of these right-inverses is a homomorphism, a consequence of—in fact, equivalent to—the fact that (2.16) does not split.) In [14, Theorem 3.3] it was shown that

$$\mathcal{E}_X = \{(U(P_{s(\pi)} R)^{-1}, \pi \cdot D) : R \in G_D, \pi \in S_p\}. \quad (2.30)$$

For  $\sigma \in \mathcal{I}_p$  and  $\pi \in S_p$ , since  $I_\sigma$  is a diagonal matrix, equations (2.23) and (2.22) implies that  $I_\sigma P_\pi = P_\pi I_{\pi^{-1} \cdot \sigma}$ . Hence if  $(\sigma, \pi) \in \tilde{S}_p^+$ ,  $D \in \text{Diag}^+(p)$ , and  $R_1 \in G_D = G_{J_D}$ , we have

$$I_\sigma P_\pi R_1 = I_{s_1(\pi)} I_{s_1(\pi)\sigma} P_\pi R_1 = I_{s_1(\pi)} P_\pi I_{\pi^{-1} \cdot (s_1(\pi)\sigma)} R_1 = P_{s(\pi)} R_2,$$

where  $R_2 = I_{\pi^{-1} \cdot (s_1(\pi)\sigma)} R_1$ . Since  $(\sigma, \pi) \in \tilde{S}_p^+$ , we have  $\text{sgn}(\sigma) = \text{sgn}(\pi) = \text{sgn}(s_1(\pi))$ , so  $s_1(\pi)\sigma \in \mathcal{I}_p^+$ , and  $\pi_1 \cdot (s_1(\pi)\sigma) \in \mathcal{I}_p^+$  for any  $\pi_1 \in S_p$ . Therefore  $I_{\pi^{-1} \cdot (s_1(\pi)\sigma)} \in \mathcal{I}_p^+$ , so  $R_2 \in G_D$  by Lemma 2.15. Since  $U(I_\sigma P_\pi R_1)^{-1} = U(P_{s(\pi)} R_2)^{-1}$ , it follows that the right-hand side of (2.27) is contained in the right-hand side of (2.30). The opposite inclusion is trivial. ■

**Corollary 2.17** *Let  $X \in \text{Sym}^+(p)$  and  $(U, D) \in \mathcal{E}_X$ . Then*

$$\mathcal{E}_X = \{(UR(P_g)^{-1}, \pi_g \cdot D) : R \in G_D^0, g \in \tilde{S}_p^+\}. \quad (2.31)$$

**Proof:** Clearly the right-hand side of (2.31) is contained in the right-hand side of (2.27), so it suffices to prove the opposite inclusion.

Let  $R \in G_D, g \in \tilde{S}_p^+$ . Enumerate the blocks of  $J := J_D$  as  $J_1, \dots, J_r$ , and let  $W_i$  be as in Definition 2.4. As noted in Remark 2.11, the enumeration of the blocks of  $J$  yields a 1-1 correspondence between  $\mathcal{I}_r^+$  and the connected components of  $G_J$ . Let  $R$  lie in the component of  $G_J$  labeled by  $(\epsilon_1, \dots, \epsilon_r) \in \mathcal{I}_r^+$ . The cardinality of  $\{j : \epsilon_j = -1\}$  is some even number  $k$ . Let  $\sigma = (\sigma_1, \dots, \sigma_p) \in \mathcal{I}_p$ , where for  $1 \leq i \leq p$  we set

$$\sigma_i = \begin{cases} -1 & \text{if } i \in J_j, \epsilon_j = -1, \text{ and } i \text{ is the smallest element of } J_j; \\ 1 & \text{otherwise.} \end{cases}$$

Then  $R_1 := I_\sigma R \in G_J^0$ . But also  $|\{i : \sigma_i = -1\}| = k$ , so  $\sigma \in \mathcal{I}_p^+ \subset \tilde{S}_p^+$ , and  $P_g I_\sigma = P_{g_1}$  for some  $g_1 \in \tilde{S}_p^+$  with  $\pi_{g_1} = \pi_g$ . Hence  $P_g R = (P_g I_\sigma)(I_\sigma R) = P_{g_1} R_1$ , so

$$(U(P_g R)^{-1}, \pi_g \cdot D) = (U(P_{g_1} R_1)^{-1}, \pi_{g_1} \cdot D),$$

which lies in the right-hand side of (2.31). The desired inclusion follows. ■

We will need a bit more notation to complete our characterization of the fibers of  $F$ :

**Notation 2.18**

1. For  $J = \{J_1, \dots, J_r\} \in \text{Part}(\{1, \dots, p\})$ , let  $K_J = \{\pi \in S_p : \pi(J_i) = J_i, 1 \leq i \leq r\}$ ,  $\Gamma_J = \tilde{S}_p^+ \cap G_J$ , and  $\Gamma_J^0 = \Gamma_J \cap G_J^0 = \tilde{S}_p^+ \cap G_J^0$ . Also define the subgroup

$$\mathcal{I}_J^+ = \{(\sigma_1, \dots, \sigma_p) \in \mathcal{I}_p : \prod_{j \in J_i} \sigma_j = 1, 1 \leq i \leq r\} \subset \mathcal{I}_p^+. \quad (2.32)$$

2. For any  $X \in \text{Sym}^+(p)$  and  $(U, D) \in \mathcal{E}_X$ , define

$$[(U, D)] = \{(UR, D) : R \in G_D^0\}, \quad (2.33)$$

the connected component of  $\mathcal{E}_X$  containing  $(U, D)$ . We write  $\text{Comp}(\mathcal{E}_X)$  for the set of connected components of  $\mathcal{E}_X$ .

3. For any Lie group  $G$  and closed subgroup  $K$ , we write  $G/K$  and  $K \backslash G$  for the spaces of left- and right-cosets, respectively, of  $K$  in  $G$ . (In particular, we use this notation when  $G$  is a finite group.)

Note that the groups  $\mathcal{I}_J^+$  are a generalization of  $\mathcal{I}_p^+$ ; for  $J = J_{\text{top}} = \{\{1\}, \{2\}, \dots, \{p\}\}$  we have  $\mathcal{I}_J^+ = \mathcal{I}_p^+$ .

We observe that equivalent definitions of  $\Gamma_J$  and  $\Gamma_J^0$  are:

$$\Gamma_J = \{(\sigma, \pi) \in \tilde{S}_p^+ : \pi \in K_J\}, \quad (2.34)$$

$$\Gamma_J^0 = \{(\sigma, \pi) \in \tilde{S}_p^+ : \sigma \in \mathcal{I}_J^+, \pi \in K_J\}. \quad (2.35)$$

Thus, analogously to (2.16), we have short exact sequences

$$1 \rightarrow \mathcal{I}_p^+ \rightarrow \Gamma_J \rightarrow K_J \rightarrow 1, \quad (2.36)$$

$$1 \rightarrow \mathcal{I}_J^+ \rightarrow \Gamma_J^0 \rightarrow K_J \rightarrow 1, \quad (2.37)$$

and the cardinality of the middle group in each of these sequences is the product of the cardinalities of the groups to its left and right. Note also that equivalent definitions of  $K_J$  are

$$\begin{aligned} K_J &= \{\pi \in S_p \mid \pi \cdot D = D \text{ for some } D \text{ with } J_D = J\} \\ &= \{\pi \in S_p \mid \pi \cdot D = D \text{ for all } D \text{ with } J_D = J\}. \end{aligned} \quad (2.38)$$

Next, observe that the group  $\tilde{S}_p^+$  acts on  $M$  via setting

$$g \cdot (U, D) = (UP_g^{-1}, g \cdot D). \quad (2.39)$$

This action preserves every fiber of  $F$ . Thus for each  $X \in \text{Sym}^+(p)$  there is an induced action of  $\tilde{S}_p^+$  on  $\text{Comp}(\mathcal{E}_X)$ , given by

$$g \cdot [(U, D)] = [g \cdot (U, D)]. \quad (2.40)$$

This leads us to:

**Proposition 2.19** *Let  $X \in \text{Sym}^+(p)$ . Then every  $(U, D) \in \mathcal{E}_X$  determines a bijection between  $\text{Comp}(\mathcal{E}_X)$  and the set  $\tilde{S}_p^+/\Gamma_{J_D}^0$ .*

**Proof:** Two elements  $(U, D), (U', D')$  lie in the same component of  $\mathcal{E}_X$  if and only if and only if  $D' = D$  and  $U' = UR$  for some  $R \in G_D^0$ . Thus it is clear from (2.31) that the action (2.40) of  $\tilde{S}_p^+$  on  $\text{Comp}(\mathcal{E}_X)$  is transitive. Therefore for any  $(U, D) \in \mathcal{E}_X$ , the map  $\tilde{S}_p^+ \rightarrow \text{Comp}(\mathcal{E}_X), g \mapsto g \cdot [(U, D)]$ , induces a bijection  $\tilde{S}_p^+/\text{Stab}([(U, D)]) \rightarrow \text{Comp}(\mathcal{E}_X)$ , where  $\text{Stab}([(U, D)])$  is the stabilizer of  $[(U, D)]$  under the action (2.40). But

$$\begin{aligned} \text{Stab}([(U, D)]) &= \{g \in \tilde{S}_p^+ \mid (UP_g^{-1}, \pi_g \cdot D) \in [(U, D)]\} \\ &= \{g \in \tilde{S}_p^+ \mid \pi_g \cdot D = D \text{ and } P_g \in G_D^0\} \\ &= \Gamma_{J_D} \cap G_{J_D}^0 \\ &= \Gamma_{J_D}^0. \end{aligned}$$

■

An important special case of Proposition 2.19 is the case in which all eigenvalues of  $X$  are distinct. In this case,  $J_D = J_{\text{top}} = \{\{1\}, \{2\}, \dots, \{p\}\}$  and  $\Gamma_{J_D}^0 = \{\text{id.}\}$ . Thus action of  $\tilde{S}_p^+$  on  $\text{Comp}(\mathcal{E}_X)$  is free as well as transitive. Furthermore  $G_D^0 = \{I\}$ , so each connected component of  $\mathcal{E}_X$  is a single point;  $\text{Comp}(\mathcal{E}_X) = \mathcal{E}_X$ . Thus  $\mathcal{E}_X$  itself is an orbit of  $\tilde{S}_p^+$ , and any choice of  $(U, D) \in \mathcal{E}_X$  yields a bijection  $\tilde{S}_p^+ \rightarrow \mathcal{E}_X$ ,  $g \mapsto g \cdot (U, D)$ .

**Corollary 2.20** *Let  $X \in \text{Sym}^+(p)$ ,  $(U, D) \in \mathcal{E}_X$ , and let  $k_1, \dots, k_r$  be the parts of the partition  $[J_D]$  of  $p$ . Then  $\mathcal{E}_X$  is diffeomorphic to a disjoint union of  $2^{r-1} \frac{p!}{k_1!k_2!\dots k_r!}$  copies of  $SO(k_1) \times SO(k_2) \times \dots \times SO(k_r)$ .*

**Proof:** Let  $J = J_D$ . It is clear from (2.33) that each connected component of  $\mathcal{E}_X$  is a submanifold of  $M$  diffeomorphic to  $G_D^0 = G_J^0$ , which from (2.6) is isomorphic (hence diffeomorphic) to  $SO(k_1) \times SO(k_2) \times \dots \times SO(k_r)$ . From Proposition 2.19, the number of connected components is  $|\tilde{S}_p^+/\Gamma_{J_D}^0| = |\tilde{S}_p^+|/|\Gamma_{J_D}^0|$ . From (2.19) we have  $|\tilde{S}_p^+| = 2^{p-1}p!$ , while from (2.37) we have  $|\Gamma_{J_D}^0| = |\mathcal{I}_J^+| |K_J|$ . It is easily seen that  $\mathcal{I}_J^+$  is isomorphic to  $(\mathbf{Z}_2)^{p-r}$ , and that  $K_J$  is isomorphic to  $S_{k_1} \times S_{k_2} \times \dots \times S_{k_r}$ , and hence that  $|K_J| = k_1!k_2!\dots k_r!$ . The result follows. ■

**Remark 2.21** An alternative, instructive route to Corollary 2.20 is the following. (We merely sketch the ideas; the reader may fill in the details.) For  $J \in \text{Part}(\{1, \dots, p\})$ , define  $\mathcal{Q}_J = \{P_g R : g \in \tilde{S}_p^+, R \in G_J\} \subset SO(p)$ . Thus the set  $\mathcal{Q}_J$  is a finite union of left-cosets of  $G_J$ , each of which is diffeomorphic to the compact submanifold  $G_J \subset SO(p)$ . If  $X \in \text{Sym}^+(p)$ ,  $(U, D) \in \mathcal{E}_X$ , and  $J = J_D$ , the map  $\mathcal{Q}_J \rightarrow M$ ,  $Q \mapsto (UQ^{-1}, QDQ^{-1})$ , is an embedding with image  $\mathcal{E}_X$ . Hence  $\mathcal{E}_X$  is a submanifold of  $M$  diffeomorphic to  $\mathcal{Q}_J$ . But for any closed subgroups  $H_1, H_2$  of a compact Lie group  $G$ , the set  $H_1 H_2 := \{h_1 h_2 : h_1 \in H_1, h_2 \in H_2\} \subset G$  is a submanifold of  $G$  and a principal  $H_2$ -bundle over  $H_1/(H_1 \cap H_2)$ , with projection map given by  $h_1 h_2 \mapsto h_1(H_1 \cap H_2)$ . Applying this to the case  $H_1 = \tilde{S}_p^+$ ,  $H_2 = G_J$ ,  $G = SO(p)$ , we have  $H_1 \cap H_2 = \Gamma_J$ , so  $\mathcal{Q}_J$  is a principal  $G_J$ -bundle over the finite set  $\tilde{S}_p^+/\Gamma_J$ . But the natural map  $\tilde{S}_p^+/\Gamma_J \rightarrow S_p/K_J$ ,  $g\Gamma_J \mapsto \text{proj}_2(g)K_J$ , is a bijection, so  $\mathcal{Q}_J$  may be viewed as a principal  $G_J$ -bundle over  $S_p/K_J$ . The cardinality of this base-space is  $|S_p|/|K_J|$ , which is simply the multinomial coefficient  $\frac{p!}{k_1!k_2!\dots k_r!}$  if  $[J] = (k_1, \dots, k_r) \in \text{Part}(p)$ . Thus  $\mathcal{E}_X$  is diffeomorphic to  $\frac{p!}{k_1!k_2!\dots k_r!}$  copies of  $G_J$ , and each copy of  $G_J$  is diffeomorphic to  $2^{r-1}$  copies of  $SO(k_1) \times \dots \times SO(k_r)$ .

### 3. Stratification of $\text{Sym}^+(p)$ , $M$ , and related spaces

The compact Lie group  $G = SO(p)$  acts from the left on the manifold  $\text{Sym}^+(p)$  via

$$(U, X) \mapsto U \cdot X = UXU^T. \quad (3.1)$$

For each  $X \in \text{Sym}^+(p)$ , the orbit  $G \cdot X$  of  $X$  is diffeomorphic to  $G/G_X$ , where  $G_X \subset G$  is the stabilizer subgroup of  $X$ :

$$G_X := \{U \in G : UXU^T = X\}. \quad (3.2)$$

If  $Y \in G \cdot X$  then  $G_Y = UG_XU^{-1}$  for any  $U$  for which  $Y = U \cdot X$ ; hence  $G_Y$  is conjugate to  $G_X$ . More generally, whether or not  $X, Y \in \text{Sym}^+(p)$  lie in the same orbit, we say that  $X$  and  $Y$  have the *same orbit type* if the stabilizers  $G_X, G_Y$  are conjugate subgroups of  $G$  (i.e. if  $G_Y = UG_XU^{-1}$  for some  $U \in G$ , an equivalence relation we will write as  $G_X \sim_c G_Y$ ). If  $X$  and  $Y$  have the same orbit type then the orbits  $G \cdot X, G \cdot Y$  are diffeomorphic. Define the *orbit-type stratum* of  $\text{Sym}^+(p)$  associated with a given orbit-type to be the union of all orbits of that type; we refer to the collection  $\mathbf{S}$  of these strata as the *orbit-type stratification* of  $\text{Sym}^+(p)$ .

The pair  $(\text{Sym}^+(p), \mathbf{S})$  is an example of a *Whitney stratified manifold*, one of several notions of “stratified space” in the literature. In all such notions, a stratification of a topological space  $Z$  is a collection  $\mathbf{S}$  of pairwise disjoint subsets of  $Z$ , called *strata*, whose union is  $Z$  and which are required to satisfy certain conditions that depend on which notion of “stratified space” is being used. The “nicest” type of stratification of a manifold is a *Whitney stratification* [10, Section 1.1]. It is known that, for any compact Lie group acting on a smooth manifold, the orbit-type stratification is a Whitney stratification ([8, p. 21]).

However, not all the criteria for a Whitney stratification are relevant to this paper. Slightly modifying the terminology of [10], the notion of greatest relevance here is that of a  *$\mathcal{P}$ -decomposed space*, where  $(\mathcal{P}, \leq)$  is a partially ordered set. A  *$\mathcal{P}$ -decomposition* of a closed subset  $Z$  of a manifold  $N$  is a locally finite collection  $\mathbf{S} = \{S_i\}_{i \in \mathcal{P}}$  of pairwise disjoint submanifolds of  $N$  whose union is  $Z$  and for which  $S_i \cap \overline{S_j} \neq \emptyset \iff S_i \subset \overline{S_j} \iff i \leq j$ , where “overbar” denotes closure. For the purposes of this paper, we allow “*stratified space*” to mean simply a  *$\mathcal{P}$ -decomposition*  $\mathbf{S}$  of a closed subset  $Z$  of some manifold, where  $\mathcal{P}$  is any partially ordered set; the submanifolds  $S_i$  are called the *strata* of this stratification. To be a Whitney stratification,  $\mathbf{S}$  must satisfy the *Whitney regularity conditions* [8, 10], technical conditions that entail “smooth attachments” of the strata. Although the orbit-type stratification of  $\text{Sym}^+(p)$  (under the action (3.1)) satisfies the Whitney regularity conditions, none of our results make use of this fact; hence our less formal use of the stratification terminology. We will, however, make pervasive use of the “ *$\mathcal{P}$ -decomposition*” notion. Our  $\mathcal{P}$  will always be either  $\text{Part}(p)$  or  $\text{Part}(\{1, \dots, p\})$ , and we will refer to it as a *label set*.

### 3.1. Three equivalent stratifications of $\text{Sym}^+(p)$

There are three “types” that we will associate to each  $X \in \text{Sym}^+(p)$ . The first, already defined, is the *orbit type* of  $X$  under the action (3.1). The other two types, *fiber type* and *eigenvalue-multiplicity type*, will be defined below. For any of these types, “ $X$  has the same type as  $Y$ ” is an equivalence relation. We



will see that all three relations are identical. Thus the orbit-type stratification may be thought of just as well as a fiber-type stratification or as an eigenvalue-multiplicity-type stratification.

First, in view of Corollary 2.20, we say that  $X, Y \in \text{Sym}^+(p)$  have the same fiber type if  $[J_D] = [J_\Lambda]$ , since under this condition the fibers  $\mathcal{E}_X, \mathcal{E}_Y$  are diffeomorphic.

Next, for  $X \in \text{Sym}^+(p)$ , we define the *eigenvalue-multiplicity type* of  $X$ , which we will denote  $\text{ET}(X)$ , to be the multi-set of multiplicities of eigenvalues of  $X$  (the collection of eigenvalues of  $X$ , enumerated with their multiplicities), an element of  $\text{Part}(p)$ . For example, if  $p = 3$ , then for any  $R_1, R_2, R_3 \in SO(3)$ , the matrices

$$X_1 = R_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 6 \end{bmatrix} R_1^{-1}, \quad X_2 = R_2 \begin{bmatrix} 4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} R_2^{-1}, \quad X_3 = R_3 \begin{bmatrix} 5 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 5 \end{bmatrix} R_3^{-1} \quad (3.3)$$

in  $\text{Sym}^+(3)$  all have the same eigenvalue-multiplicity type, the partition  $2 + 1$  of 3. The relative *sizes* of the eigenvalues of  $X \in \text{Sym}^+(p)$  have no bearing on the eigenvalue-multiplicity type of  $X$ ; all that matters are the eigenvalue *multiplicities*. As we shall see later, in our stratification of  $\text{Diag}^+(p)$  the three diagonal matrices in (3.3) represent two different strata.

The three “types” we have defined are conceptually different: For  $X \in \text{Sym}^+(p)$  and  $D \in \text{Diag}^+(p)$  for which  $(U, D) \in \mathcal{E}_X$  for some  $U \in SO(p)$ ,

- (i) the concept of *orbit-type* is based on (though not necessarily equivalent to) diffeomorphism type of the *orbit*  $G \cdot X$ , a connected submanifold of  $\text{Sym}^+(p)$  diffeomorphic to  $SO(p)/G_D$ , hence of dimension  $\dim(SO(p)) - \dim(G_D^0)$  (cf. [17, Lemma 4.1]);
- (ii) the concept of *fiber-type* of  $X$  is based on (though not necessarily equivalent to) the diffeomorphism type of the *fiber*  $\mathcal{E}_X$ , a possibly non-connected submanifold of  $SO(p) \times \text{Diag}^+(p)$  diffeomorphic to finitely many copies of  $G_D$  (the number of copies being the multinomial coefficient  $\frac{p!}{k_1! \dots k_r!}$  appearing in Corollary 2.20), hence of dimension  $G_D$ ; and
- (iii) the concept of *eigenvalue-multiplicity type* is based directly on discrete information: the partition  $[J_D]$  of  $p$  determined by the eigenvalues of  $X$ .

But now let  $X, Y \in \text{Sym}^+(p)$ ,  $(U, D) \in \mathcal{E}_X$ , and  $(V, \Lambda) \in \mathcal{E}_Y$ . Note that  $G_X \sim_c G_D$  and  $G_Y \sim_c G_\Lambda$ . Hence

$$\begin{aligned} X, Y \text{ have the same orbit-type} &\iff G_X \sim_c G_Y \\ &\iff G_D \sim_c G_\Lambda \\ &\iff J_D = \pi \cdot J_\Lambda \quad \text{for some } \pi \in S_p \\ &\iff [J_D] = [J_\Lambda] \\ &\iff \text{ET}(X) = \text{ET}(Y). \end{aligned}$$

Thus, for all  $X, Y \in \text{Sym}^+(p)$ ,

$$\text{same orbit-type} = \text{same fiber-type} = \text{same eigenvalue-multiplicity type}, \quad (3.4)$$

even though the three kinds of “types” are conceptually different.

Because of (3.4), we are free to view the orbit-type stratification as an eigenvalue-multiplicity-type stratification, and to label strata accordingly. We will do this in Section 3.2.

### 3.2. Four stratified spaces

We use  $\text{Part}(\{1, \dots, p\})$  to define stratifications of the spaces  $\text{Diag}^+(p)$  and  $M = (SO \times \text{Diag}^+)(p)$ , and use  $\text{Part}(p)$  to define stratifications of  $\text{Diag}^+(p)/S_p$  and  $\text{Sym}^+(p)$ . The commutative diagram in Figure 1 indicates the relationships among these spaces and label-sets. In this diagram, the maps not yet defined are as follows:

$$\begin{array}{ccccc}
 M = SO(p) \times \text{Diag}^+(p) & \xrightarrow{\text{proj}_2} & \text{Diag}^+(p) & \xrightarrow{\text{lbl}} & \text{Part}(\{1, \dots, p\}) \\
 \downarrow F & & \downarrow \text{quo}_1 & & \downarrow \text{quo}_2 \\
 \text{Sym}^+(p) & \xrightarrow{\overline{\text{proj}_2}} & \text{Diag}^+(p)/S_p & \xrightarrow{\overline{\text{lbl}}} & \text{Part}(p)
 \end{array}$$

FIG 1. Commutative diagram defining the stratifications of  $\text{Sym}^+(p)$  and related spaces.

- $\text{proj}_2 : SO(p) \times \text{Diag}^+(p) \rightarrow \text{Diag}^+(p)$  is projection onto the second factor.
- For  $X \in \text{Sym}^+(p)$ , if  $(U, D) \in \mathcal{E}_X$  we define  $\overline{\text{proj}_2}(X) = [D] \in \text{Sym}^+(p)/S_p$ ; this is well-defined since in any two eigen-decompositions  $X$ , the diagonal parts differ at most by a permutation.
- The stratum-labeling map  $\text{lbl} : \text{Diag}^+(p) \rightarrow \text{Part}(\{1, \dots, p\})$  is defined by  $\text{lbl}(D) = J_D$ .
- The stratum-labeling map  $\overline{\text{lbl}} : \text{Diag}^+(p) \rightarrow \text{Part}(p)$  is defined by  $\overline{\text{lbl}}([D]) = [J_D]$ .
- $\text{quo}_1$  and  $\text{quo}_2$  are the quotient maps  $\text{Diag}^+(p) \rightarrow \text{Diag}^+(p)/S_p$  and  $\text{Part}(\{1, \dots, p\}) \rightarrow \text{Part}(\{1, \dots, p\})/S_p = \text{Part}(p)$  respectively.

We define strata as the diagram suggests: for  $J \in \text{Part}(\{1, \dots, p\})$  and  $[K] \in \text{Part}(p)$ ,

$$\begin{aligned}
\mathcal{D}_J &:= \text{lbl}^{-1}(J) = \{D \in \text{Diag}^+(p) : J_D = J\} \subset \text{Diag}^+(p), \\
\mathcal{D}_{[K]} &:= \overline{\text{lbl}}^{-1}([K]) = \{[D] \in \text{Diag}^+(p)/S_p : \pi \cdot D \in \mathcal{D}_K \text{ for some } \pi \in S_p\} \\
&\quad \subset \text{Diag}^+(p)/S_p, \\
\mathcal{S}_J &:= \text{proj}_2^{-1}(\mathcal{D}_J) = SO(p) \times \mathcal{D}_J \\
&= \{(U, D) \in M : J_D = J\} \subset M, \\
\mathcal{S}_{[K]} &:= \overline{\text{proj}_2}^{-1}(\mathcal{D}_{[K]}) = \{X \in \text{Sym}^+(p) \text{ with eigenvalue-multiplicity type } [K]\} \\
&= \{X \in \text{Sym}^+(p) : X = F(U, D) \text{ for some} \\
&\quad U \in SO(p), D \in \mathcal{D}_K\} \subset \text{Sym}^+(p).
\end{aligned}$$

For example, the matrices  $X_1, X_2, X_3$  in (3.3) all lie in the same stratum  $\mathcal{S}_{[J]}$  of  $\text{Sym}^+(p)$ , the one labeled by the partition  $[J] = 2+1$  of 3. The diagonal matrices  $D_1, D_2, D_3$  appearing in the formulas in (3.3) for  $X_1, X_2, X_3$ , respectively, lie in two different strata of  $M$ : the first two lie in  $\mathcal{D}_{J_1}$  while the third lies in  $\mathcal{D}_{J_2}$ , where  $J_1 = \{\{2, 3\}, \{1\}\}$  and  $J_2 = \{\{1, 3\}, \{2\}\}$ . Note that strata need not be connected. For example, the stratum  $\mathcal{S}_{2+1}$  in  $\text{Sym}^+(3)$  has two connected components, one in which the double-eigenvalue is the larger of the two distinct eigenvalues, and one in which it is the smaller. The matrix  $X_1$  in (3.3) lies in the first of these components, while  $X_2$  and  $X_3$  lie in the second. The diagonal matrices  $D_1$  and  $D_2$  lie in different connected components of  $\mathcal{D}_{J_1}$ .

It is clear that each of the four spaces  $\text{Diag}^+(p)$ ,  $M$ ,  $\text{Diag}^+(p)/S_p$ , and  $\text{Sym}^+(p)$ , is the disjoint union of the strata we have defined in that space. Note also that for any  $J \in \text{Part}(\{1, \dots, p\})$ ,  $F(\mathcal{S}_J) = \mathcal{S}_{[J]}$  and  $\text{quo}_1(\mathcal{D}_J) = \mathcal{D}_{[J]}$ .

If  $J, K \in \text{Part}(\{1, \dots, p\})$  and  $K$  is a strict refinement of  $J$  (i.e.  $K$  refines  $J$  but  $K \neq J$ ; equivalently,  $J < K$ ), it is easy to see that every element of the stratum  $\mathcal{S}_J$  in  $M$  can be obtained as a limit of a sequence lying in  $\mathcal{S}_K$ , but that no element of  $\mathcal{S}_K$  can be obtained as a limit of a sequence lying in  $\mathcal{S}_J$  (in the limit of a sequence of matrices, distinct eigenvalues can coalesce but equal eigenvalues cannot separate). A similar comment applies to strata  $\mathcal{D}_J, \mathcal{D}_K$  in  $\text{Diag}^+(p)$ ; to strata  $\mathcal{S}_{[J]}, \mathcal{S}_{[K]}$  in  $\text{Sym}^+(p)$ ; and to strata  $\mathcal{D}_{[J]}, \mathcal{D}_{[K]}$  in  $\text{Diag}^+(p)/S_p$ .

$$\overline{\mathcal{D}_K} = \bigcup_{J \leq K} \mathcal{D}_J, \quad \overline{\mathcal{S}_K} = \bigcup_{J \leq K} \mathcal{S}_J, \quad (3.5)$$

$$\overline{\mathcal{D}_{[K]}} = \bigcup_{[J] \leq [K]} \mathcal{D}_{[J]}, \quad \overline{\mathcal{S}_{[K]}} = \bigcup_{[J] \leq [K]} \mathcal{S}_{[J]}. \quad (3.6)$$

The map  $\text{diag}(d_1, \dots, d_p) \rightarrow (d_1, \dots, d_p)$ , identifies  $\text{Diag}^+(p)$  diffeomorphically with  $(\mathbf{R}_+)^p$ . Under this identification, for each  $J \in \text{Part}(\{1, \dots, p\})$  the stratum  $\mathcal{D}_J$  is the intersection of a linear subspace of  $\mathbf{R}^p$  with the open subset  $(\mathbf{R}_+)^p \subset \mathbf{R}^p$ , hence is a submanifold of  $(\mathbf{R}_+)^p$ . The stratum  $\mathcal{S}_J = SO(p) \times \mathcal{D}_J$  is therefore a submanifold of  $M$ . The quotient  $\text{Diag}^+(p)/S_p$  is simply the  $p$ -fold symmetric product of  $\mathbf{R}_+$ , which can be identified homeomorphically with

$Z := \{(x_1, \dots, x_p) \in (\mathbf{R}_+)^p : x_1 \leq x_2 \leq \dots \leq x_p\}$ , a closed subset of  $(\mathbf{R}_+)^p$ . This homeomorphism identifies the stratum  $\mathcal{D}_{[J]}$  of  $\text{Diag}^+(p)/S_p$  with a submanifold of  $(\mathbf{R}_+)^p$  (diffeomorphic to a connected component of  $\mathcal{D}_J$ ). Thus our collections of strata of  $\text{Diag}^+(p)$ ,  $\text{Diag}^+(p)/S_p$ , and  $M$  meet our definition of “stratified space”. As noted earlier, our stratification of  $\text{Sym}^+(p)$  is an orbit-type stratification, hence automatically a Whitney stratification. Thus, each of  $\text{Diag}^+(p)$ ,  $M$ ,  $\text{Diag}^+(p)/S_p$ , and  $\text{Sym}^+(p)$ , equipped with the strata defined above, is a stratified space.

For any stratified space, we define a partial ordering “ $\leq$ ” on the set of strata  $\mathcal{T}_i$  by declaring  $\mathcal{T}_1 \leq \mathcal{T}_2$  if  $\mathcal{T}_1 \subset \overline{\mathcal{T}_2}$ . Then (3.5)–(3.6) imply that for all  $J, K \in \text{Part}(\{1, \dots, p\})$ , in the appropriate spaces we have

$$\mathcal{S}_J \leq \mathcal{S}_K \iff J \leq K \iff \mathcal{D}_J \leq \mathcal{D}_K, \quad (3.7)$$

$$\mathcal{S}_{[J]} \leq \mathcal{S}_{[K]} \iff [J] \leq [K] \iff \mathcal{D}_{[J]} \leq \mathcal{D}_{[K]}. \quad (3.8)$$

(It is for this reason that we defined the partial orders on  $\text{Part}(\{1, \dots, p\})$  and  $\text{Part}(p)$  to be of the form “parent  $\leq$  child” rather than the more natural-looking “child  $\leq$  parent.”) In each of the stratified spaces above, there is a highest stratum and a lowest stratum namely the strata labeled by  $J_{\text{top}}$ ,  $[J_{\text{top}}]$ ,  $J_{\text{bot}}$ , and  $[J_{\text{bot}}]$ . Note that for  $J, K \in \text{Part}(\{1, \dots, p\})$ ,  $J \leq K$  implies  $[J] \leq [K]$ , but the converse is false for  $p > 2$ . In view of (3.7)–(3.8), a similar comment applies to our stratified spaces:  $\mathcal{S}_J \leq \mathcal{S}_K$  implies  $\mathcal{S}_{[J]} \leq \mathcal{S}_{[K]}$ , and  $\mathcal{D}_J \leq \mathcal{D}_K$  implies  $\mathcal{D}_{[J]} \leq \mathcal{D}_{[K]}$ , but the converse of each of these implications is false for  $p > 2$ .

**Remark 3.1 (Number of strata)** The number of strata of  $\text{Sym}^+(p)$  is the number of partitions of  $p$ , while the number of strata of  $M$  is the number of partitions of  $\{1, \dots, p\}$ . In number theory, the *partition function* is the function that assigns to each positive integer  $n$  the number partitions of  $n$ . The number of partitions of  $\{1, \dots, n\}$  is known as the  $n^{\text{th}}$  *Bell number*. Both the partition function and the Bell numbers have a long history and have been extensively studied; see [12, Chapter XIX], [18].

**Remark 3.2 (Dimensions of strata)** The dimensions of the strata in each of the four stratified spaces in diagram (1) can easily be worked out; we will simply state the answers. If  $J \in \text{Part}(\{1, \dots, p\})$  and  $[J] = (k_1, \dots, k_r)$ , then

$$\begin{aligned} \dim(\mathcal{S}_J) &= r + \dim(SO(p)) = r + \frac{p(p-1)}{2}, \\ \dim(\mathcal{S}_{[J]}) &= r + (\dim(SO(p)/G_J)) = r + (\dim(SO(p)) - \dim(G_J^0)) \\ &= r + \frac{p(p-1)}{2} - \sum_{i=1}^r \frac{k_i(k_i-1)}{2}, \quad \text{and} \\ \dim(\mathcal{D}_J) &= \dim(\mathcal{D}_{[J]}) = r. \end{aligned}$$

### 3.3. Examples

Using Corollary 2.20 and Remarks 3.2 and 3.1, for any given  $p$  we can, in principle, describe all the fibers of  $F$  and all the strata of  $M$  and  $\text{Sym}^+(p)$  very

explicitly. As  $p$  grows, the number of strata and the number of diffeomorphism-types of fibers grows rapidly, so below we do this exercise only for the cases  $p = 2$  and  $p = 3$ .

### 3.3.1. Example: $\text{Sym}^+(2)$

**Stratification of  $M$  and  $\text{Diag}^+(2)$ .** There are two strata of  $M = (SO \times \text{Diag}^+)(2)$  (and of  $\text{Diag}^+(2)$ ), labeled by the two partitions of  $\{1, 2\}$ :  $J_{\text{top}} = \{\{1\}, \{2\}\}$  and  $J_{\text{bot}} = \{\{1, 2\}\}$ .

- (a) The two-dimensional stratum  $\mathcal{D}_{J_{\text{top}}}$  consists of two connected components,  $\{\text{diag}(d_1, d_2) : d_1 > d_2 > 0\}$  and  $\{\text{diag}(d_1, d_2) : d_2 > d_1 > 0\}$ . Correspondingly, the three-dimensional stratum  $\mathcal{S}_{J_{\text{top}}} = SO(2) \times \mathcal{D}_{J_{\text{top}}}$  also has two connected components.
- (b) The one-dimensional stratum  $\mathcal{D}_{J_{\text{bot}}}$  is the connected set  $\{\text{diag}(d_1, d_2) : d_1 = d_2 > 0\}$ . Therefore the two-dimensional stratum  $\mathcal{S}_{J_{\text{bot}}} = SO(2) \times \mathcal{D}_{J_{\text{bot}}}$  is also connected.

In the top panels of Figure 2,  $\mathcal{S}_{J_{\text{bot}}}$  (respectively,  $\mathcal{D}_{J_{\text{bot}}}$ ) is schematically depicted as the green plane (resp., line), which separates the two connected components of  $\mathcal{S}_{J_{\text{top}}}$  (resp.,  $\mathcal{D}_{J_{\text{top}}}$ ).

**Stratification of  $\text{Sym}^+(2)$  and  $\text{Diag}^+(2)/S_2$ .** There are two strata of  $\text{Sym}^+(2)$  (and of  $\text{Diag}^+(2)/S_2$ ), corresponding to the two partitions of 2:  $[J_{\text{top}}] = 1+1$ , and  $[J_{\text{bot}}] = 2$ . It is easily checked that for any  $J \in \text{Part}(\{1, \dots, p\})$ ,  $F(\mathcal{S}_J) = \mathcal{S}_{[J]}$ ,  $\text{quo}_1(\mathcal{D}_J) = \mathcal{D}_{[J]}$ .

- (a) The top stratum  $\mathcal{S}_{[J_{\text{top}}]} = \mathcal{S}_{1+1}$  is three-dimensional and consists of SPD matrices with two distinct eigenvalues. Unlike  $\mathcal{S}_{J_{\text{top}}}$  in  $M$ , the stratum  $\mathcal{S}_{[J_{\text{top}}]}$  in  $\text{Sym}^+(2)$  is connected. In the bottom left panel of Figure 2,  $\mathcal{S}_{[J_{\text{top}}]}$  corresponds to the inside of the cone, minus the green line.
- (b) The bottom stratum  $\mathcal{S}_{[J_{\text{bot}}]} = \mathcal{S}_2$  is one-dimensional and consists of SPD matrices with only one distinct eigenvalue. This stratum is depicted as the green line in Figure 2.

**Fibers of  $X \in \text{Sym}^+(2)$ .** The fibers are characterized by Corollary 2.20.

- (a) For any  $X \in \mathcal{S}_{[J_{\text{top}}]} = \mathcal{S}_{1+1}$ , the fiber  $\mathcal{E}_X \subset \mathcal{S}_{J_{\text{top}}} \subset M$  consists of four points.
- (b) For any  $X \in \mathcal{S}_{[J_{\text{bot}}]} = \mathcal{S}_2$ , the fiber  $\mathcal{E}_X \subset \mathcal{S}_{J_{\text{bot}}} \subset M$  is diffeomorphic to a circle. An example of this circle is depicted schematically as the red line segment in the top left panel of Figure 2.

### 3.3.2. Example: $\text{Sym}^+(3)$

**Stratification of  $M$  and  $\text{Diag}^+(3)$ .** There are six strata of  $M = (SO \times \text{Diag}^+)(3)$  (and of  $\text{Diag}^+(3)$ ), labeled by the six partitions of  $\{1, 2, 3\}$ ; See Ta-

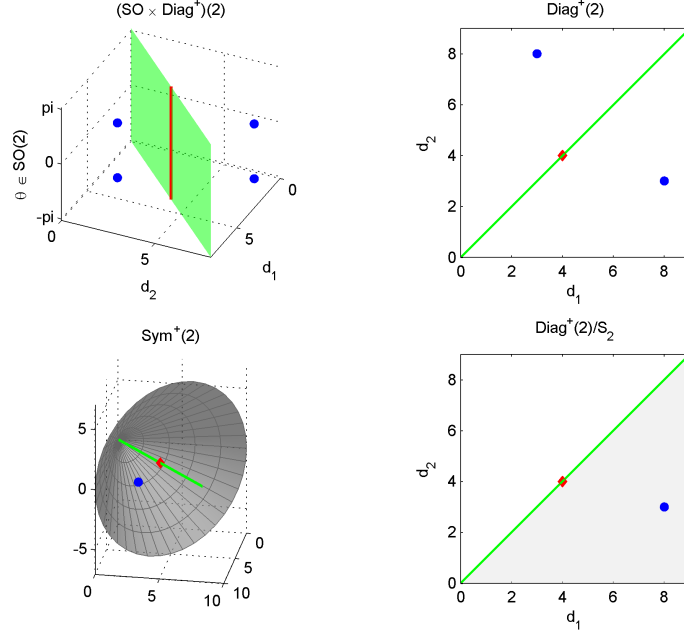


FIG 2. Stratification of  $M = (SO \times \text{Diag}^+)(2)$  (top left),  $\text{Sym}^+(2)$  (bottom left),  $\text{Diag}^+(2)$  (top right) and  $\text{Diag}^+(2)/S_2$  (shaded area in bottom right).  $\text{Sym}^+(2)$  is embedded in  $\text{Sym}(2) \cong \mathbf{R}^3$  as the cone  $\{(a_{11}, a_{22}, \sqrt{2}a_{12}) : a_{11} > 0, a_{22} > 0, a_{11}a_{22} - a_{12}^2 > 0\}$ . The space  $\text{Diag}^+(2)/S_2$  is represented as a fundamental domain for the action of  $S_2$  on  $\text{Diag}^+(2)$  (a subset  $A \subset \text{Diag}^+(2)$  containing exactly one point of each orbit, and such that  $\text{quo}_1 : \text{Diag}^+(2) \rightarrow \text{Diag}^+(2)/S_2$  restricts to a homeomorphism  $\text{quo}_1^{-1}(A \setminus \partial A) \rightarrow A \setminus \partial A$ ). Also shown are  $X = \text{diag}(8, 3) \in \mathcal{S}_{[\text{J}_{\text{top}}]} \subset \text{Sym}^+(2)$  (blue dot) and  $Y = \text{diag}(4, 4) \in \mathcal{S}_{[\text{J}_{\text{bot}}]}$  (red dot), as well as their pre-images in  $M$ . The projections to  $\text{Diag}^+(2)$  and  $\text{Diag}^+(2)/S_2$  of these subsets of  $M$  and  $\text{Sym}^+(2)$  are illustrated as correspondingly-colored dots in the right-hand panels.

ble 1. The features of the stratum  $\mathcal{D}_J$  we discuss below apply to the corresponding stratum  $\mathcal{S}_J = SO(3) \times \mathcal{D}_J$ .

- (a) The stratum  $\mathcal{D}_{J_{\text{bot}}}$  is the connected component  $\{\text{diag}(d_1, d_2, d_3) : d_1 = d_2 = d_3\}$ . In the top panel of Figure 3,  $\mathcal{D}_{J_{\text{bot}}}$  corresponds to the green line.
- (b) The stratum  $\mathcal{D}_{J_1}$  consists of two connected components:  $\mathcal{D}_{J_1}^{\text{pro}} = \{\text{diag}(d_1, d_2, d_3) : d_1 > d_2 = d_3\}$  and  $\mathcal{D}_{J_1}^{\text{ob}} = \{\text{diag}(d_1, d_2, d_3) : d_1 < d_2 = d_3\}$ . (The superscripts “pro” and “ob” stand for “prolate” and “oblate”, respectively; see below.) The closures of these two connected components intersect in  $\mathcal{D}_{J_{\text{bot}}}$ . In Figure 3,  $\mathcal{D}_{J_1}$  corresponds to one of the three shaded planes except the green line. The stratum  $\mathcal{S}_{J_1}$  also consists of two connected components:  $\mathcal{S}_{J_1}^{\text{pro}} = SO(3) \times \mathcal{D}_{J_1}^{\text{pro}}$  and  $\mathcal{S}_{J_1}^{\text{ob}} = SO(3) \times \mathcal{D}_{J_1}^{\text{ob}}$ . The

strata  $\mathcal{D}_{J_i}$  and  $\mathcal{S}_{J_i}$  for  $i = 2$  and  $3$  are similarly characterized.

- (c) The stratum  $\mathcal{D}_{J_{\text{top}}}$  consists of six connected components, which can be labeled by permutations of  $\{1, 2, 3\}$ . Precisely,  $\mathcal{D}_{J_{\text{top}}} = \bigcup_{\pi \in S_3} \mathcal{D}_{J_{\text{top}}}^\pi$ , where  $\mathcal{D}_{J_{\text{top}}}^\pi = \{\text{diag}(d_1, d_2, d_3) : d_{\pi^{-1}(1)} > d_{\pi^{-1}(2)} > d_{\pi^{-1}(3)}\}$  for  $\pi \in S_3$ .

**Stratification of  $\text{Sym}^+(3)$  and  $\text{Diag}^+(3)/S_3$ .** There are three strata of  $\text{Sym}^+(3)$  (and of  $\text{Diag}^+(3)/S_3$ ), corresponding to the three partitions of 3:  $[J_{\text{top}}] = 1 + 1 + 1$ ,  $[J_{\text{mid}}] = 2 + 1$ , and  $[J_{\text{bot}}] = 3$ . These stratifications are closely related to an ellipsoid classification. An SPD matrix  $X \in \text{Sym}^+(3)$  with eigenvalues  $a \geq b \geq c$  corresponds to the ellipsoid given by the equation  $x^T X^{-1} x = 1$ , and has the shape of a sphere if  $a = b = c$ , an oblate spheroid if  $a = b > c$ , a prolate spheroid if  $a > b = c$ , or a tri-axial ellipsoid if  $a > b > c$ . We will say that  $X \in \text{Sym}^+(3)$  is prolate (respectively oblate, triaxial) if the corresponding ellipsoid is a prolate spheroid (resp. oblate spheroid, triaxial ellipsoid).

- (a) The stratum  $\mathcal{S}_{[J_{\text{top}}]} = \mathcal{S}_{1+1+1}$  is the set of all SPD matrices with three distinct eigenvalues. Every  $X \in \mathcal{S}_{[J_{\text{top}}]}$  is tri-axial. In the bottom panel of Figure 3, the corresponding stratum  $\mathcal{D}_{[J_{\text{top}}]} \subset \text{Diag}^+(3)$  is depicted as an open convex cone.  $\mathcal{S}_{[J_{\text{top}}]}$  is connected.
- (b) The stratum  $\mathcal{S}_{[J_{\text{mid}}]} = \mathcal{S}_{2+1}$  consists of SPD matrices with just two distinct eigenvalues, and is a disjoint union of two connected components:  $\mathcal{S}_{2+1}^{\text{pro}} = F(\mathcal{S}_{J_1}^{\text{pro}})$  and  $\mathcal{S}_{2+1}^{\text{ob}} = F(\mathcal{S}_{J_1}^{\text{ob}})$ . If  $X \in \mathcal{S}_{2+1}^{\text{pro}}$ , then  $X$  is prolate; if  $X \in \mathcal{S}_{2+1}^{\text{ob}}$ , then  $X$  is oblate. Likewise, the stratum  $\mathcal{D}_{2+1}$  is a disjoint union of two connected components:  $\mathcal{D}_{2+1}^{\text{ob}}$  and  $\mathcal{D}_{2+1}^{\text{pro}}$ . In the bottom left panel of Figure 3, the two gray open planar sectors represent these two connected components of  $\mathcal{D}_{2+1}$ .
- (c) The stratum  $\mathcal{S}_{[J_{\text{bot}}]} = \mathcal{S}_3$  is the set of all SPD matrices with only one distinct eigenvalue. The corresponding ellipsoids have the shape of a sphere.  $\mathcal{S}_{[J_{\text{bot}}]}$  is connected.

**Fibers of  $X \in \text{Sym}^+(3)$ .**

- (a) For any  $X \in \mathcal{S}_{[J_{\text{top}}]} = \mathcal{S}_{1+1+1}$ , the fiber  $\mathcal{E}_X \subset M$  consists of 24 points, all of which lie in  $\mathcal{S}_{J_{\text{top}}} \in M$ .
- (b) For any  $X \in \mathcal{S}_{[J_{\text{mid}}]} = \mathcal{S}_{2+1}$ , the fiber  $\mathcal{E}_X \subset M$  is diffeomorphic to 6 copies of the circle.
- (c) For any  $X \in \mathcal{S}_{[J_{\text{bot}}]} = \mathcal{S}_3$ , the fiber  $\mathcal{E}_X \subset \mathcal{S}_{J_{\text{bot}}} \subset M$  is diffeomorphic to (one copy of)  $SO(3)$  (and thus to  $\mathbf{R}P^3$ ).

In Figure 3, examples of the three types of fibers are provided. To help visualize, we show the projected fibers,  $\text{proj}_2(\mathcal{E}_X) \subset \text{Diag}^+(3)$ . (For any  $X \in \mathcal{S}_{k_1+\dots+k_r} \subset \text{Sym}^+(p)$ ,  $\text{proj}_2(\mathcal{E}_X)$  is a discrete set of cardinality  $\frac{p!}{k_1!k_2!\dots k_r!}$ .)

#### 4. Scaling-rotation distance and minimal smooth scaling-rotation curves

The Lie groups  $SO(p)$  and  $\text{Diag}^+(p)$  carry natural bi-invariant Riemannian metrics. If we endow  $M = SO(p) \times \text{Diag}^+(p)$  with a product Riemannian metric

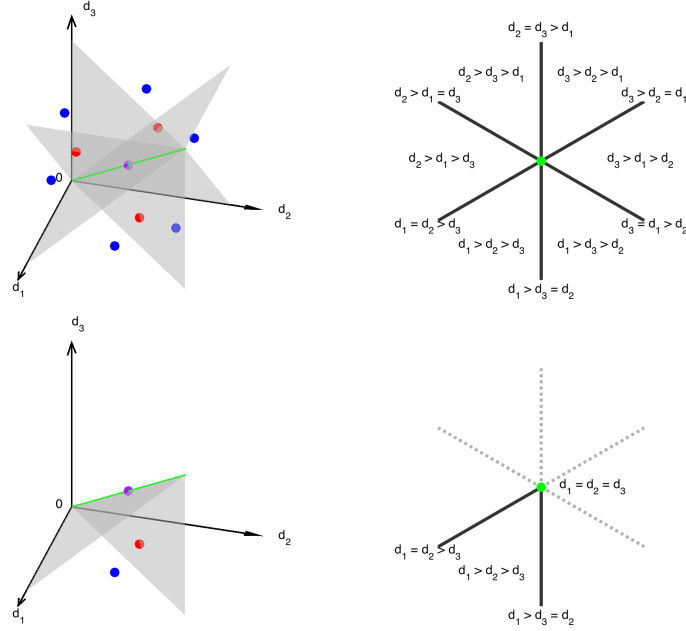


FIG 3. Stratification of  $\text{Diag}^+(3)$  (top left) and  $\text{Diag}^+(3)/S_3$  (bottom left). The star-figure (top right) represents the intersection of the top left figure and a hyperplane orthogonal to the green line. In the bottom left panel, the space  $\text{Diag}^+(3)/S_3$  is represented as a fundamental domain for the action of  $S_3$  on  $\text{Diag}^+(3)$ , a convex cone bounded by below by the positive quadrant of the  $d_1d_2$ -plane and on the sides by the two indicated gray planar sectors. Since the spaces  $\text{Sym}^+(3)$  and  $M = (SO \times \text{Diag}^+)(3)$  are six-dimensional, there are no simple visualizations of them. Also shown are projections of  $X = \text{diag}(8, 5, 1) \in \mathcal{S}_{[\text{top}]} \subset \text{Sym}^+(3)$  (blue dot),  $Y = \text{diag}(6, 6, 2) \in \mathcal{S}_{[\text{mid}]}$  (red dot), and  $Z = \text{diag}(5, 5, 5) \in \mathcal{S}_{[\text{bot}]}$  (green dot) to  $\text{Diag}^+(3)/S_3$  (bottom) and the pre-images of the quotient map in  $\text{Diag}^+(3)$  (top).

$g_M$  (allowing a constant weighting-factor  $k$ ), the geodesics  $\gamma$  in  $(M, g_M)$  are easily computed. We define *smooth scaling-rotation (SSR) curves* in  $\text{Sym}^+(p)$  to be the projections to  $\text{Sym}^+(p)$  of the geodesics in  $(M, g_M)$ , i.e. curves of the form  $F \circ \gamma$ . (In [16] and [14] these were called simply “scaling-rotation curves”. Remark 4.7 explains why we have added “smooth” to this name.)

#### 4.1. Smooth scaling-rotation curves

The Lie algebra  $\mathfrak{so}(p) = T_I(SO(p))$  is the space of  $p \times p$  antisymmetric matrices. For  $U \in SO(p)$ , the tangent space  $T_U(SO(p))$  can be identified with either the left-translate or right-translate of  $\mathfrak{so}(p) = T_I(SO(p))$  by  $U$ . For the purposes of



this paper the latter identification is somewhat more convenient:

$$T_U(SO(p)) = \{AU : A \in SO(p) : A \in \mathfrak{so}(p)\}. \quad (4.1)$$

With this identification, the standard bi-invariant Riemannian metric  $g_{SO(p)}$  on  $SO(p)$  is defined by

$$g_{SO(p)}|_U(A_1, A_2) = -\frac{1}{2}\mathrm{tr}(A_1U^{-1}A_2U^{-1}), \quad (4.2)$$

where  $U \in SO(p)$  and  $A_1, A_2 \in T_U(SO(p))$ . (The requirement of bi-invariance determines the metric  $g_{SO(p)}$  up to a constant factor unless  $p = 4$ ; the fact that the Lie-algebra  $\mathfrak{so}(4)$  is a direct sum of two copies of the simple Lie algebra  $\mathfrak{so}(3)$  leads to a two-parameter family of bi-invariant metrics on  $SO(4)$ .)

The open set  $\mathrm{Diag}^+(p)$  is also a Lie group, but since it is an open set of  $\mathrm{Diag}(p)$  we make the identification  $T_D(\mathrm{Diag}^+(p)) = T_D(\mathrm{Diag}(p))$  for all  $D \in \mathrm{Diag}^+(p)$ . This abelian Lie group carries a (bi-)invariant Riemannian metric  $g_{\mathcal{D}^+}$  defined by

$$g_{\mathcal{D}^+}|_D(L_1, L_2) = \mathrm{tr}(D^{-1}L_1D^{-1}L_2) \quad (4.3)$$

where  $D \in \mathrm{Diag}^+(p)$  and  $L_1, L_2 \in T_U(SO(p))$ . There is a  $p$ -parameter family of bi-invariant metrics on  $\mathrm{Diag}^+(p)$ , but, up to a constant factor,  $g_{\mathcal{D}^+}$  is the unique one that is also invariant under the action of the symmetric group  $S_p$ .

On  $M := SO(p) \times \mathrm{Diag}^+(p)$ , we will use a product Riemannian metric determined by the metrics on the two factors. Specifically, letting  $k > 0$  be an arbitrary parameter that can be chosen as desired for applications, we set

$$g_M|_{(U,D)}((A_1, L_1), (A_2, L_2)) = k g_{SO(p)}|_U(A_1, A_2) + g_{\mathcal{D}^+}|_D(L_1, L_2), \quad (4.4)$$

where  $U \in SO(p)$ ,  $D \in \mathrm{Diag}^+(p)$ , and  $(A_i, L_i) \in T_U(SO(p)) \oplus T_D(\mathrm{Diag}^+(p)) = T_{(U,D)}M$ . Since the metrics  $g_{SO(p)}$  and  $g_{\mathcal{D}^+}$  are bi-invariant, the geodesics in  $M$  can be obtained as either left-translates or right-translates of geodesics through the identity  $(I, I)$ . In this paper, the latter will be more convenient.

**Definition 4.1** A *smooth scaling-rotation (SSR) curve* is a curve  $\chi$  in  $\mathrm{Sym}^+(p)$  of the form  $F \circ \gamma$ , where  $\gamma : I \rightarrow M$  is a geodesic defined on some interval  $I$ .

Note: in this paper, we use *curve* sometimes to mean a *parametrized curve*—a map  $I \rightarrow Z$ , where  $I$  is an interval and  $Z$  is some space—and sometimes to mean an equivalence class of such maps, where two maps are regarded as equivalent if one is a monotone reparametrization of the other. (In particular, two such equivalent maps have the same image.) It should always be clear from context which meaning is intended.

**Notation 4.2** For  $(U, D) \in M$ ,  $A \in SO(p)$ ,  $L \in \mathrm{Diag}(p)$ , and  $I \subset \mathbf{R}$  an interval, we define  $\gamma_{U,D,A,L} : \mathbf{R} \rightarrow M$  and  $\chi_{U,D,A,L} : \mathbf{R} \rightarrow \mathrm{Sym}^+(p)$  by

$$\gamma_{U,D,A,L}(t) = (\exp(tA)U, \exp(tL)D) \quad (4.5)$$

and

$$\chi_{U,D,A,L} = F \circ \gamma_{U,D,A,L}. \quad (4.6)$$

We use the same notation  $\gamma_{U,D,A,L}$ ,  $\chi_{U,D,A,L}$  for the restrictions of the curves above to any interval  $I \subset \mathbf{R}$ .

The curve  $\gamma_{U,D,A,L} : \mathbf{R} \rightarrow M$  is the geodesic in  $M$  with initial conditions  $\gamma(0) = (U, D)$ ,  $\gamma'(0) = (AU, DL) \in T_{(U,D)}M$ . The projection of  $\gamma_{U,D,A,L}$  to  $\text{Sym}^+(p)$ , the curve  $\chi_{U,D,A,L}$ , is the corresponding smooth scaling-rotation curve.

Recall that in any group  $G$ , an element  $g$  is called an *involution* if  $g^2$  is the identity element  $e$  but  $g \neq e$ . Thus  $R \in SO(p)$  is an involution if  $R^2 = I \neq R$ . The cut-locus of the identity in  $SO(p)$  is precisely the set of all involutions. For every non-involution  $R \in SO(p)$ , there is a unique  $A \in \mathfrak{so}(p)$  of smallest norm such that  $\exp(A) = R$  (see Section 7.1); we define  $\log(R) = A$ . If  $R$  is an involution, there is more than one smallest-norm  $A \in \mathfrak{so}(p)$  such that  $\exp(A) = R$ , and we allow  $\log(R)$  to denote the *set* of all such  $A$ 's. However, all elements  $A$  in this set have the same norm, which we write as  $\|\log(R)\|$ . Thus  $\|\log(R)\|$  is a well-defined real number for all  $R \in SO(p)$ , even though  $\log(R)$  is not a unique element of  $\mathfrak{so}(p)$  when  $R$  is an involution. With this understood, the geodesic-distance function  $d_M$  on  $M$  is given by

$$d_M^2((U, D), (V, \Lambda)) = k d_{SO(p)}(U, V)^2 + d_{\mathcal{D}^+}(D, \Lambda)^2 \quad (4.7)$$

$$= \frac{k}{2} \|\log(U^{-1}V)\|^2 + \|\log(D^{-1}\Lambda)\|^2, \quad (4.8)$$

where in (4.8) and for the rest of this paper,  $\|\cdot\|$  denotes the Frobenius norm on matrices:  $\|A\|^2 = \|A\|_F^2 = \text{tr}(A^T A)$  for any matrix  $A$ .

The invariances of the metrics  $d_{SO(p)}$  and  $d_{\mathcal{D}^+}$  lead to the following:

**Proposition 4.3** ([14, Proposition 3.7]) *The geodesic distance (4.7) on  $M$  is invariant under simultaneous left or right multiplication by orthogonal matrices, permutations and scaling: For any  $R_1, R_2 \in O(p)$ ,  $\pi \in S_p$  and  $S \in \text{Diag}^+(p)$ , and for any  $(U, D), (V, \Lambda) \in (SO \times \text{Diag}^+)(p)$ ,*

$$d_M((U, D), (V, \Lambda)) = d_M((R_1 U R_2, S \pi \cdot D), (R_1 V R_2, S \pi \cdot \Lambda)).$$

#### 4.2. Scaling-rotation distance and MSSR curves

**Definition 4.4** ([14, Definition 3.10]) For  $X, Y \in \text{Sym}^+(p)$ , the *scaling-rotation distance*  $d_{\mathcal{SR}}(X, Y)$  between  $X$  and  $Y$  is defined by

$$d_{\mathcal{SR}}(X, Y) := \inf_{\substack{(U,D) \in \mathcal{E}_X, \\ (V,\Lambda) \in \mathcal{E}_Y}} d_M((U, D), (V, \Lambda)). \quad (4.9)$$

**Definition 4.5** Let  $\gamma$  be a piecewise-smooth curve in  $M$  and let  $\ell(\gamma)$  denote the length of  $\gamma$ . For  $X, Y \in \text{Sym}^+(p)$ , we call  $\gamma : [0, 1] \rightarrow M$  an  $(\mathcal{E}_X, \mathcal{E}_Y)$ -*minimal geodesic* if  $\gamma(0) \in \mathcal{E}_X$ ,  $\gamma(1) \in \mathcal{E}_Y$ , and  $\ell(\gamma) = d_{\mathcal{SR}}(X, Y)$ . We call a pair of points  $((U, D), (V, \Lambda)) \in \mathcal{E}_X \times \mathcal{E}_Y$  a *minimal pair* if  $(U, D) = \gamma(0)$  and  $(V, \Lambda) = \gamma(1)$  for some  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesic  $\gamma$ . A *minimal smooth scaling-rotation* (MSSR)

curve from  $X$  to  $Y$  is a curve  $\chi$  in  $\text{Sym}^+(p)$  of the form  $F \circ \gamma$  where  $\gamma$  is an  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesic. We say that the MSSR curve  $\chi = F \circ \gamma$  *corresponds* to the minimal pair formed by the endpoints of  $\gamma$ . We let  $\mathcal{M}(X, Y)$  denote the set of MSSR curves from  $X$  to  $Y$ .

Obviously an  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesic is a minimal geodesic in the usual sense of Riemannian geometry: it is a curve of shortest length among all piecewise-smooth curves with the same endpoints. From the general theory of geodesics (see e.g. [5]), any such curve  $\gamma$  is actually *smooth*, and, when parametrized at constant speed, satisfies the geodesic equation  $\nabla_{\gamma'} \gamma' \equiv 0$ . Thus a definition equivalent to (4.9) is

$$d_{\mathcal{SR}}(X, Y) = \inf \{ \ell(\gamma) \mid \gamma : [0, 1] \rightarrow M \text{ is a geodesic with } \gamma(0) \in \mathcal{E}_X, \gamma(1) \in \mathcal{E}_Y \}. \quad (4.10)$$

Thus an  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesic can alternatively be defined as a geodesic of minimal length among all geodesics starting in  $\mathcal{E}_X$  and ending in  $\mathcal{E}_Y$ .

From Corollary 2.20, every fiber of  $F$  is compact, so the infimum in (4.9) is always achieved. Hence for all  $X, Y \in \text{Sym}^+(p)$ , there always exists an  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesic, a minimal pair in  $\mathcal{E}_X \times \mathcal{E}_Y$ , and an MSSR curve from  $X$  to  $Y$ . We discuss uniqueness issues in the next subsection.

**Remark 4.6** Observe that we have not defined a Riemannian metric on  $\text{Sym}^+(p)$ , so there is no “automatic” meaning attached to the phrase *length of a smooth curve* in  $\text{Sym}^+(p)$ . However, for an SSR curve  $\chi$  in  $\text{Sym}^+(p)$  we define the *length of  $\chi$*  to be  $\ell(\chi) := \inf \{ \ell(\gamma) : \gamma \text{ is a geodesic in } M \text{ and } F \circ \gamma = \chi \}$ . With this definition, (4.10) becomes

$$d_{\mathcal{SR}}(X, Y) = \inf \{ \ell(\chi) \mid \chi : [0, 1] \rightarrow \text{Sym}^+(p) \text{ is an SSR curve with } \chi(0) = X, \chi(1) = Y \}. \quad (4.11)$$

**Remark 4.7** As noted in [14], the “scaling-rotation distance”  $d_{\mathcal{SR}}$  is *not* a metric on  $\text{Sym}^+(p)$ ; it does not satisfy the triangle inequality. In [11], we use the function  $d_{\mathcal{SR}}$  to construct a true scaling-rotation metric  $\rho_{\mathcal{SR}}$  on  $\text{Sym}^+(p)$ . Effectively, the construction enlarges the class of scaling-rotation (SR) curves  $\chi$  considered in (4.11) from smooth curves to piecewise-smooth curves (with  $\ell(\chi)$  redefined correspondingly); hence the word “smooth” in Definition 4.1. (It is not trivial to show that the corresponding infimum  $\rho_{\mathcal{SR}}(X, Y)$  is nonzero for  $X \neq Y$ .) This definition of  $\rho_{\mathcal{SR}}$  is analogous to the definition of “distance between two points in a Riemannian manifold”: the infimum of the lengths of *piecewise-smooth* curves joining the points. Some minimal-length scaling-rotation curves are non-smooth; an MSSR curve from  $X$  to  $Y$  has minimal length only among *smooth* SR curves from  $X$  to  $Y$ . This phenomenon does not occur in Riemannian geometry; in a Riemannian manifold, minimal piecewise-smooth curves between two points are actually *smooth*.

**Definition 4.8** Recall that given any group  $G$  and subgroups  $H_1, H_2$ , an  $(H_1, H_2)$  *double-coset* is an equivalence class under the equivalence relation  $\sim$  on  $G$  defined by declaring  $g_1 \sim g_2$  if there exist  $h_1 \in H_1, h_2 \in H_2$  such that  $g_2 = h_1 g_1 h_2$ .

The set of equivalence classes under this relation is denoted  $H_1 \backslash G / H_2$ . By a *set of representatives* of  $H_1 \backslash G / H_2$  we mean a subset of  $G$  consisting of exactly one element from each  $(H_1, H_2)$  double-coset. Note that every ordinary left coset or right coset is also a double coset (with the second subgroup taken to be trivial), so “set of representatives” is defined for ordinary cosets as well.

In Sections 5 and 6 we will apply the next proposition to compute all scaling-rotation distances, and to help compute and classify all smooth minimal scaling-rotation curves, in the case  $p = 3$ . For the definition of  $\Gamma_{\mathcal{D}}^0$  see Notation 2.18 or (2.35).

**Proposition 4.9** *Let  $X, Y \in \text{Sym}^+(p)$  and let  $(U, D) \in \mathcal{E}_X, (V, \Lambda) \in \mathcal{E}_Y$ . Let  $Z$  be any set of representatives of  $\Gamma_{\mathcal{D}}^0 \backslash \tilde{S}_p^+ / \Gamma_{\Lambda}^0$ . Then the scaling-rotation distance from  $X$  to  $Y$  is given by*

$$d_{\mathcal{SR}}(X, Y)^2 = \min \left\{ k d_{SO(p)}(UR_U, VR_V P_g^{-1})^2 + d_{\mathcal{D}^+}(D, \pi_g \cdot \Lambda) \right\}^2 : \quad (4.12)$$

$$R_U \in G_{\mathcal{D}}^0, R_V \in G_{\Lambda}^0, \text{ and } g \in Z$$

$$= \min_{g \in Z} \left\{ k \left( \min \left\{ d_{SO(p)}(UR_U, VR_V P_g^{-1})^2 : R_U \in G_{\mathcal{D}}^0, R_V \in G_{\Lambda}^0 \right\} \right)^2 + \left\| \log(D^{-1}(\pi_g \cdot \Lambda)) \right\|^2 \right\}. \quad (4.13)$$

Every minimal smooth scaling-rotation curve from  $X$  to  $Y$  corresponds to some minimal pair whose first element lies in the connected component  $[(U, D)]$  of  $\mathcal{E}_X$ . A pair  $((UR_U, D), (VR_V P_g^{-1}, \pi_g \cdot \Lambda))$  with  $R_U \in G_{\mathcal{D}}^0, R_V \in G_{\Lambda}^0$ , and  $g \in \tilde{S}_p^+$ , is minimal if and only if the triple  $(g, R_U, R_V)$  is a minimizer of the expression in braces in (4.12).

**Proof:** From Proposition 2.16, we have

$$\mathcal{E}_X \times \mathcal{E}_Y = \left\{ (UR_U P_{g_1}^{-1}, \pi_{g_1} \cdot D), (VR_V P_{g_2}^{-1}, \pi_{g_2} \cdot \Lambda) : R_U \in G_{\mathcal{D}}^0, R_V \in G_{\Lambda}^0; g_1, g_2 \in \tilde{S}_p^+ \right\}. \quad (4.14)$$

Using Proposition 4.3 and the fact the maps  $g \mapsto \pi_g, g \mapsto P_g$ , are homomorphisms, for all  $g_1, g_2 \in \tilde{S}_p^+$  we have

$$d((UR_U P_{g_1}^{-1}, \pi_{g_1} \cdot D), (VR_V P_{g_2}^{-1}, \pi_{g_2} \cdot \Lambda)) \quad (4.15)$$

$$= d((UR_U, D), (VR_V (P_{g_1^{-1}g_2})^{-1}, \pi_{g_1^{-1}g_2} \cdot \Lambda)). \quad (4.16)$$

The map  $(\tilde{U}, \tilde{D}) \mapsto (\tilde{U} P_{g_1}, \pi_{g_1}^{-1} \cdot \tilde{D})$  underlying the equality above is an isometry of  $(SO \times \text{Diag}^+)(p)$  that preserves every fiber, hence carries a geodesic  $\gamma_1$  with the endpoints in (4.15) into a geodesic  $\gamma_2$  with the endpoints in (4.16) and that satisfies  $F \circ \gamma_1 = F \circ \gamma_2$ . Hence, every smooth scaling-rotation (SSR) curve from  $X$  to  $Y$  is of the form  $F \circ \gamma$  where  $\gamma : [0, 1] \rightarrow (SO \times \text{Diag}^+)(p)$  is a geodesic with  $\gamma(0) = (UR_U, D) \in [(U, D)]$  and  $\gamma(1) \in \mathcal{E}_Y$ .

Suppose  $\gamma_1, \gamma_2$  are two such geodesics, with  $\gamma_i(1) = (VR_V P_{g_i}^{-1}, \pi_{g_i} \cdot \Lambda)$ ,  $i = 1, 2$ . If  $g_2 = h_D g_1 h_\Lambda$ , with  $h_D \in \Gamma_{J_D}^0$  and  $h_\Lambda \in \Gamma_{J_\Lambda}^0$ , then

$$\begin{aligned} d((UR_U, D), (VR_V P_{g_2}^{-1}, \pi_{g_2} \cdot \Lambda)) \\ &= d((UR_U, D), (VR_V h_\Lambda^{-1} P_{g_1}^{-1} h_D^{-1}, \pi_{h_D} \cdot \pi_{g_1} \cdot \pi_{h_\Lambda} \cdot \Lambda)) \\ &= d((UR_U h_D, \pi_{h_D} \cdot D), (VR_V h_\Lambda^{-1} P_{g_1}^{-1}, \pi_{g_1} \cdot \pi_{h_\Lambda} \cdot \Lambda)) \\ &= d((UR_{U,1}, D), (VR_{V,1} P_{g_1}^{-1}, \pi_{g_1} \cdot \Lambda)) \end{aligned}$$

where  $R_{U,1} = R_U h_D \in G_D^0$  and  $R_{V,1} = R_V h_\Lambda^{-1} \in G_\Lambda^0$ . The same argument as in the preceding paragraph shows that the SSR curve determined by the pair  $((UR_U, D), (VR_V P_{g_2}^{-1}, \pi_{g_2} \cdot \Lambda))$  is the same as the SSR curve determined by the pair  $((UR_{U,1}, D), (VR_{V,1} P_{g_1}^{-1}, \pi_{g_1} \cdot \Lambda))$ . Hence any representative  $g \in \tilde{S}_p^+$  of a given  $(\Gamma_{J_D}^0, \Gamma_{J_\Lambda}^0)$  double-coset determines the same set of SSR curves (the set of curves  $F \circ \gamma$ , where  $\gamma$  is a geodesic from  $(UR_U, D)$  to  $(VR_V g^{-1}, \pi_g \cdot \Lambda)$  for some  $R_U \in G_D^0, R_V \in G_\Lambda^0$ ) as does any other representative of that double-coset. The Proposition now follows.  $\blacksquare$

Proposition 4.9 remains true if  $Z$  is replaced by  $\tilde{S}_p^+$  in (4.12), or by a set of representatives of the left-coset space  $S_p/\Gamma_{J_\Lambda}^0$  or the right-coset space  $\Gamma_{J_D}^0 \backslash S_p$ . However, taking  $Z$  as in the Proposition reduces the combinatorial complexity of the minimization problem when the eigenvalues of  $X$  or  $Y$  are not all distinct. For example, when  $p = 3$ , we will see in Section 5.2.1 that when  $X$  and  $Y$  both have exactly two distinct eigenvalues, there are only three  $(\Gamma_{J_D}^0, \Gamma_{J_\Lambda}^0)$  double-cosets, whereas there are six left  $\Gamma_{J_\Lambda}^0$ -cosets and six right  $\Gamma_{J_D}^0$ -cosets, and 24 elements of  $\tilde{S}_p^+$ .

### 4.3. Uniqueness questions for MSSR curves

As noted in Section 4.1, for all  $X, Y \in \text{Sym}^+(p)$  there always exists an MSSR curve from  $X$  to  $Y$ , the projection of some  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesic. *A priori*, different  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesics could project to the same MSSR curve or to different MSSR curves. It is natural to ask: Under what conditions on  $(X, Y)$  is there a unique MSSR curve from  $X$  to  $Y$ ? When uniqueness fails, *how* does it fail, and what can we say about the set  $\mathcal{M}(X, Y)$ ?

For uniqueness to fail for given  $X, Y$ , there must be distinct  $(\mathcal{E}_X, \mathcal{E}_Y)$ -minimal geodesics  $\gamma_i : [0, 1] \rightarrow M$ , whose endpoints are minimal pairs  $((U_i, D_i), (V_i, \Lambda_i)) \in \mathcal{E}_X \times \mathcal{E}_Y$ ,  $i = 1, 2$ , such that  $F \circ \gamma_1 \neq F \circ \gamma_2$ . The “how” question above concerns the following two possibilities (not mutually exclusive):

1. “Type I non-uniqueness”: There exist such  $\gamma_i$  whose endpoints are *distinct* minimal pairs  $((U_i, D_i), (V_i, \Lambda_i))$ .
2. “Type II non-uniqueness”: There exist such  $\gamma_i$  whose endpoints are *the same* minimal pair  $((U, D), (V, \Lambda))$ .

Since for any  $D, \Lambda \in \text{Diag}^+(p)$  the minimal geodesic from  $D$  to  $\Lambda$  is unique, Type II non-uniqueness with minimal pair  $((U, D), (V, \Lambda))$  is equivalent to the existence of two or more minimal geodesics from  $U$  to  $V$ , which is equivalent to each of  $U, V$  being in the cut-locus (in  $SO(p)$ ) of the other. It will be convenient for us to have some other terminology for this situation:

**Definition 4.10** Call a pair of points  $(U, V)$  in  $SO(p) \times SO(p)$  *geodesically antipodal* if one point is in the cut-locus of the other (equivalently, if each point is in the cut-locus of the other) and *geodesically non-antipodal* otherwise. Call a pair of points  $((U, D), (V, \Lambda))$  in  $M \times M$  geodesically antipodal if  $(U, V)$  is a geodesically antipodal pair in  $SO(p) \times SO(p)$ , and geodesically non-antipodal otherwise.

As mentioned earlier, the cut-locus of the identity  $I \in SO(p)$  is precisely the set of all involutions in  $SO(p)$ . Furthermore, because of the invariance of the Riemannian metric  $g_{SO(p)}$ , an element  $V \in SO(p)$  is in the cut-locus of element  $U$  if and only if  $V^{-1}U$  is in the cut-locus of  $I$ . Note that, for elements  $a, b$  of any group,  $ab$  is an involution  $\iff ba$  is an involution  $\iff b^{-1}a^{-1}$  is an involution  $\iff a^{-1}b^{-1}$  is an involution. Thus, if any of the elements  $V^{-1}U, UV^{-1}, U^{-1}V, VU^{-1}$  is an involution, so are all the others.

Note that a pair  $(U, V)$  in  $SO(p)$  can be geodesically antipodal without either point being maximally remote from the other. (For example, with  $p = 4$ , the matrix  $\text{diag}(-1, -1, 1, 1)$  is an involution, but is closer to the identity  $I$  than is the involution  $-I$ .) However, if  $(U, V)$  is geodesically antipodal, then there exists a (not necessarily unique) closed geodesic in  $SO(p)$  containing  $U$  and  $V$ , isometric to a circle of some radius, such that  $U$  and  $V$  are antipodal points of this circle in the usual sense, and such that each of the two semicircles connecting  $U$  and  $V$  is a minimal geodesic between these two points.

One reason for our interest in Type II non-uniqueness is its effect on a true scaling-rotation *metric* on  $\text{Sym}^+(p)$  that we construct from  $d_{\mathcal{SR}}$  in [11]. Various constructions and assertions concerning this metric are simplified when we know that Type II non-uniqueness does not occur.

For small enough values of  $p$ , Type II non-uniqueness never occurs; for large enough  $p$ , it always occurs. The method by which we will prove these facts takes us in directions rather far from the rest of this paper, so our most precise statements and proofs are deferred to the Appendix, which also contains some results that may be of independent interest. However, we will introduce here our main tool for ruling out Type II non-uniqueness, based on a property we call *sign-change reducibility*, defined shortly.

To motivate the definition, let  $X, Y \in \text{Sym}^+(p)$  and let  $((U, D), (V, \Lambda)) \in \mathcal{E}_X \times \mathcal{E}_Y$  be a minimal pair. Then one minimizer  $(g, R_U, R_V)$  of the expression in brackets on the right-hand side of (4.12) is the triple  $(e, I, I)$ , where  $e$  is the identity element of  $\tilde{S}_p^+$ . Hence for all  $g \in \tilde{S}_p$  with  $\pi_g \cdot \Lambda = \Lambda$ —i.e. for all  $g \in K_{J_\Lambda}$  (see Notation 2.18 and equation (2.38))—we must have  $d_{SO(p)}(UP_g, V) = d_{SO(p)}(U, VP_g^{-1}) \geq d_{SO(p)}(U, V)$ . But  $\mathcal{I}_p^+ \subset K_J$  for all  $J$  (since sign-change matrices act trivially on  $\text{Diag}^+(p)$ ), so, in particular, we must have  $d_{SO(p)}(UI_\sigma, V) \geq d_{SO(p)}(U, V)$  for all  $\sigma \in \mathcal{I}_p^+$ .

**Definition 4.11** Call a pair of points  $(U, V) \in SO(p) \times SO(p)$  *sign-change reducible* if  $d_{SO(p)}(UI_{\sigma}, V) < d_{SO(p)}(U, V)$  for some  $\sigma \in \mathcal{I}_p^+$ .

From the discussion preceding Definition 4.11, we have the following:

**Corollary 4.12** *Let  $((U, D), (V, \Lambda)) \in M \times M$ . If  $(U, V) \in SO(p) \times SO(p)$  is sign-change reducible, then  $((U, D), (V, \Lambda))$  is not a minimal pair. ■*

In the Appendix we investigate sign-change reducibility in more detail. In this section we will just summarize some results proven there, and their consequences. Two of these results are in the following Proposition:

**Proposition 4.13** (a) *For  $p \leq 4$ , every geodesically antipodal pair  $(U, V)$  in  $SO(p) \times SO(p)$  is sign-change reducible.* (b) *For  $p \geq 11$ , there exist geodesically antipodal pairs  $(U, V)$  in  $SO(p) \times SO(p)$  that are not sign-change reducible.*

Thus the largest dimension  $p_1$  for which every geodesically antipodal pair  $(U, V)$  in  $SO(p_1) \times SO(p_1)$  is sign-change reducible satisfies  $4 \leq p_1 \leq 10$ . A combination of theory and numerical evidence leads the authors to believe that  $p_1$  is closer to 10 than to 4.

An immediate consequence of Proposition 4.13 (a) is:

**Corollary 4.14** *For  $p \leq 4$ , every minimal pair in  $M \times M$  is geodesically non-antipodal.*

Hence for  $p \leq 4$ , for all  $X, Y \in \text{Sym}^+(p)$  for which  $\mathcal{M}(X, Y) > 1$ , the non-uniqueness is purely of Type I. (Again, we do not believe the number “4” here is sharp.)

Also proven in the Appendix is the following:

**Proposition 4.15** *Suppose that  $(U, V)$  is a pair in  $SO(p) \times SO(p)$  that is not sign-change reducible. Then there exist  $D, \Lambda \in \mathcal{D}_{J_{\text{top}}}$  such that the pair  $((U, D), (V, \Lambda))$  is minimal.*

An immediate corollary of Propositions 4.13(b) and 4.15 is:

**Corollary 4.16** *For  $p \geq 11$ , there exist geodesically antipodal, minimal pairs  $((U, D), (V, \Lambda)) \in \mathcal{S}_{J_{\text{top}}} \times \mathcal{S}_{J_{\text{top}}} \subset M \times M$ . Hence, for  $p \geq 11$ , there exist  $X, Y \in \mathcal{S}_{J_{\text{top}}} \subset \text{Sym}^+(p)$  for which the set  $\mathcal{M}(X, Y)$  exhibits Type II non-uniqueness.*

Thus sign-change reducibility is more than an *ad hoc* criterion for ruling out Type II non-uniqueness for small enough  $p$ . Proposition 4.15 and Corollary 4.16 show that, in some sense, sign-change reducibility is the only obstruction to having points  $X, Y$  in the top stratum of  $\text{Sym}^+(p)$  for which  $\mathcal{M}(X, Y)$  exhibits Type II nonuniqueness.

For  $X$  or  $Y$  not in the top stratum of  $\text{Sym}^+(p)$ , the relationship between Type II nonuniqueness and sign-change reducibility of minimal pairs in  $\mathcal{E}_X \times \mathcal{E}_Y$  situation is more complicated to analyze. We do not investigate this relationship further in this paper.

#### 4.4. Determining the set of MSSR curves

Proposition 4.9 is a starting-point for understanding the set  $\mathcal{M}(X, Y)$  for all  $p$  and all  $X, Y \in \text{Sym}^+(p)$ . The Proposition assures us that, for any  $(U, D) \in \mathcal{E}_X$ , every MSSR curve from  $X$  to  $Y$  corresponds to some minimal pair whose first element lies in the connected component  $[(U, D)]$  of  $\mathcal{E}_X$ . In Section 6, for  $p = 3$  we will see how to find all such minimal pairs. (For the case  $p = 2$ , [14, Section 4.1] indicates how to find all minimal pairs.) But for any  $p$ , even once we know all the minimal pairs, to completely understand  $\mathcal{M}(X, Y)$ , or even just determine its cardinality, we need a way to tell whether MSSR curves corresponding to two (not necessarily distinct) minimal pairs with first point in  $[(U, D)]$  are the same. (This is true whether the non-uniqueness, if any, in  $\mathcal{M}(X, Y)$  is of Type I, Type II, or a mixture of both). The following proposition provides such a tool.

**Proposition 4.17** *Let  $X, Y \in \text{Sym}^+(p)$ ,  $X \neq Y$ . For  $i = 1, 2$  assume that  $\chi_i = F \circ \gamma_i$  is a minimal smooth scaling-rotation curve from  $X$  to  $Y$  corresponding to the minimal pair  $((UR_{U,i}, D), (VR_{V,i}P_{g_i}^{-1}, \Lambda_i))$ , where  $R_{U,i} \in G_D^0$ ,  $R_{V,i} \in G_\Lambda^0$ ,  $g_i \in \tilde{S}_p^+$ ,  $\Lambda_i = \pi_{g_i} \cdot \Lambda$ , and  $\gamma_i : [0, 1] \rightarrow M$  is a geodesic. (We do not assume that the two minimal pairs are distinct.) Then  $\chi_1 = \chi_2$  if and only if the following two conditions hold.*

- (i) *Both pairs  $(UR_{U,i}, VR_{V,i}P_{g_i}^{-1})$  are geodesically non-antipodal and*

$$R_{V,2}P_{g_2}^{-1}R_{U,2}^{-1} = R_{V,1}P_{g_1}^{-1}R_{U,1}^{-1}, \quad (4.17)$$

*or both pairs are geodesically antipodal and*

$$(\text{proj}_{SO(p)}\gamma_1'(0))R_{U,1}^{-1} = (\text{proj}_{SO(p)}\gamma_2'(0))R_{U,2}^{-1}, \quad (4.18)$$

*where for any  $(U', D') \in M$ ,  $\text{proj}_{SO(p)}$  denotes the natural projection  $T_{(U', D')}M \rightarrow T_{U'}SO(p)$ .*

- (ii) *There exist  $g \in \tilde{S}_p^+$ ,  $R \in G_{D, \Lambda_1}^0$  such that*

$$D = \pi_g \cdot D, \quad (4.19)$$

$$\Lambda_2 = \pi_g \cdot \Lambda_1, \quad (4.20)$$

$$\text{and } R_{U,1}^{-1}R_{U,2} = RP_g^{-1}. \quad (4.21)$$

Equation (4.18) implies equation (4.17), so (4.17) is always a necessary condition for the equality  $\chi_1 = \chi_2$ .

In Proposition 4.17, in the geodesically non-antipodal case we use *endpoint data* to tell whether the projections to  $\text{Sym}^+(p)$  of two minimal geodesics from  $\mathcal{E}_X$  to  $\mathcal{E}_Y$  are equal. We will deduce this proposition from the following theorem, proven in [14], that gives a criterion based on *initial-value data* to tell whether the projections of two geodesics emanating from  $\mathcal{E}_X$  are equal. In this theorem,  $G_{D,L} := G_D \cap G_L$ ,  $\mathfrak{g}_{D,L} := \mathfrak{g}_D \cap \mathfrak{g}_L$  (the Lie algebra of  $G_{D,L}$ ), and for  $A \in SO(p)$ ,  $\text{ad}_A : \mathfrak{so}(p) \rightarrow \mathfrak{so}(p)$  is the linear map defined by  $\text{ad}_A(B) = [A, B]$ .



**Theorem 4.18** ([14, Theorem 3.8]) *For  $i = 1, 2$  let  $(U_i, D_i) \in M$ ,  $A_i \in \mathfrak{so}(p)$ ,  $L_i \in \text{Diag}(p)$ , and let  $\check{A}_i = U_1^{-1}A_iU_1$ . Let  $I$  be a positive-length interval containing 0. Then the smooth scaling-rotation curves  $\chi_i := \chi_{U_i, D_i, A_i, L_i} : I \rightarrow \text{Sym}^+(p)$  are identical if and only if (i)  $\check{A}_2 - \check{A}_1 \in \mathfrak{g}_{D_1, L_1}$ , (ii)  $(\text{ad}_{\check{A}_2})^j(\check{A}_1) \in \mathfrak{g}_{D_1, L_1}$  for all  $j \geq 1$ , and (iii) there exist  $R \in G_{D_1, L_1}$  and  $g \in \tilde{S}_p^+$ , such that  $U_2 = U_1 R P_g^{-1}$ ,  $D_2 = \pi_g \cdot D_1$ , and  $L_2 = \pi_g \cdot L_1$ .<sup>1</sup>*

To deduce Proposition 4.17 from Theorem 4.18, we first prove two lemmas that may be useful beyond their roles in proving the Proposition. In these lemmas, for any  $X \in \text{Sym}^+(p)$  we write  $\mathfrak{g}_X$  for the Lie algebra of the stabilizer  $G_X$  defined in (3.2); thus  $\mathfrak{g}_X = \{A \in \mathfrak{so}(p) : AX = XA\}$ . (If  $X = D \in \text{Diag}^+(p)$  is a diagonal matrix  $D$ , then this stabilizer is the group  $G_D$  we have previously defined, and  $\mathfrak{g}_D$  is its Lie algebra.)

**Lemma 4.19** *Let  $X, Y \in \text{Sym}^+(p)$  and suppose that  $\chi : [0, 1] \rightarrow \text{Sym}^+(p)$  is a minimal smooth rotation-scaling curve with  $X := \chi(0) \neq Y := \chi(1)$ . Let  $\gamma = \gamma_{U, D, A, L} : [0, 1] \rightarrow (SO \times \text{Diag})^+(p)$  be a geodesic for which  $\chi = F \circ \gamma$ . Then  $A \in (\mathfrak{g}_X)^\perp \cap (\mathfrak{g}_Y)^\perp$ , where the orthogonal complements are taken in  $\mathfrak{so}(p)$ .*

**Proof:** Since  $\gamma$  is a smooth curve of minimal length connecting the submanifolds  $\mathcal{E}_X$  and  $\mathcal{E}_Y$  of  $(SO \times \text{Diag})^+(p)$ , the velocity vectors  $\gamma'(0), \gamma'(1)$  must be perpendicular to the tangent spaces  $T_{\gamma(0)}\mathcal{E}_X, T_{\gamma(1)}\mathcal{E}_Y$ , respectively ([5, Proposition 1.5]). Making natural tangent-space identifications, we have  $T_{\gamma(0)}\mathcal{E}_X = T_{(U, D)}\mathcal{E}_X = U\mathfrak{g}_D \oplus \{0\} \subset U\mathfrak{g}_D \oplus \text{Diag}(p)$ , where  $U\mathfrak{g}_D := \{UC : C \in \mathfrak{g}_D\}$ . Let  $\check{A} = U^{-1}AU$ . Since  $\gamma'(0) = (U\check{A}, DL)$ , and the Riemannian metric we are using on  $SO(p)$  is left-invariant, the condition  $\gamma'(0) \perp T_{\gamma(0)}\mathcal{E}_X$  is equivalent to  $\check{A} \in (\mathfrak{g}_D)^\perp$ , hence to  $A \in U(\mathfrak{g}_D)^\perp U^{-1}$ . Using additionally the right-invariance of the metric on  $\mathfrak{so}(p)$ , we have  $U(\mathfrak{g}_D)^\perp U^{-1} = (U\mathfrak{g}_D U^{-1})^\perp$ . From general group-action properties, it is easily seen that  $U\mathfrak{g}_D U^{-1} = \mathfrak{g}_{UDU^{-1}}$ . Since  $UDU^{-1} = X$ , it follows that  $A \in (\mathfrak{g}_X)^\perp$ . A similar argument at the point  $(V, \Lambda) := \gamma(1)$  shows that  $A \in (\mathfrak{g}_{V\Lambda V^{-1}})^\perp = (\mathfrak{g}_Y)^\perp$ . ■

**Lemma 4.20** *In the setting of Theorem 4.18, assume that the smooth scaling-rotation curve  $\chi_1$  is minimal. Then conditions (i) and (ii) in the theorem can be replaced by the single condition  $A_2 = A_1$ .*

**Proof:** With notation as in Theorem 4.18, assume that  $\chi_2 = \chi_1$ . Then the Theorem implies that  $U^{-1}(A_2 - A_1)U \in \mathfrak{g}_{D, L} \subset \mathfrak{g}_D$ , implying that  $A_2 - A_1 \in U\mathfrak{g}_D U^{-1} = \mathfrak{g}_X$  (as in the proof of Lemma 4.19). But since  $\chi_1$  is minimal, Lemma 4.19 implies that both  $A_2$  and  $A_1$  lie in  $(\mathfrak{g}_X)^\perp$ , hence that  $A_2 - A_1 \in (\mathfrak{g}_X)^\perp$ . Hence  $A_2 - A_1 = 0$ , i.e.  $A_2 = A_1$ .

Conversely, assume that  $A_2 = A_1$ . Then conditions (i) and (ii) are satisfied trivially. ■

<sup>1</sup>In [14, Theorem 3.8],  $g$  was actually required to be of the form  $(s(\pi), \pi)$ , where  $s$  is as in (2.29). But the same argument as in the proof of Proposition 2.16 shows that this restriction can be removed.

**Proof of Proposition 4.17:** For  $i \in \{1, 2\}$  let  $U_i = UR_{U,i}$ ,  $V_i = VR_{V,i}P_{g_i}^{-1}$ , and  $\Lambda_i = \pi_{g_i} \cdot \Lambda_i$ .

By hypothesis  $\chi_i = F \circ \gamma_i$ , where  $\gamma_i = \gamma_{U_i, D, A_i, L_i} : [0, 1] \rightarrow M$  (for some  $A_i \in \mathfrak{so}(p)$ ,  $L_i \in \text{Diag}(p)$ ) is a minimal geodesic from  $(U_i, D)$  to  $(V_i, \Lambda_i)$ . Hence  $L_i = \log(\Lambda_i D^{-1})$  and  $A_i \in \log(V_i U_i^{-1})$ . (Recall from Section 4.1 that when  $R \in SO(p)$  is not an involution, “log  $R$ ” means the unique minimal-norm element  $A \in \mathfrak{so}(p)$  such that  $\exp(A) = R$ , and when  $R$  is an involution, “log  $R$ ” means the set of all such minimal-norm elements.)

It is straightforward to show that  $G_{D, L_i} = G_{D, \Lambda_i}$ . From Lemma 4.20, the conditions (i) and (ii) in Theorem 4.18 in the equality-conditions for  $\chi_1$  and  $\chi_2$  can be replaced by the single condition  $A_2 = A_1$ .

If  $A_2 = A_1$  then  $V_2 U_2^{-1} = V_1 U_1^{-1}$ , implying that either both pairs  $\{(U_i, V_i)\}$  are geodesically antipodal or both are geodesically non-antipodal. In the converse direction, suppose that the pairs  $\{(U_i, V_i)\}$  are geodesically non-antipodal and that  $V_2 U_2^{-1} = V_1 U_1^{-1}$ . Then  $A_2 = \log(V_2 U_2^{-1}) = \log(V_1 U_1^{-1}) = A_1$ . Whether or not the pairs  $\{(U_i, V_i)\}$  are geodesically antipodal, by definition  $(\text{proj}_{SO(p)} \gamma'_i(0)) U_i^{-1} = A_i$ , so if (4.18) holds then  $A_2 = A_1$ . Hence the condition  $A_2 = A_1$  is equivalent to condition (i) in Proposition 4.17.

Next, letting  $D$  play the role of  $D_1$  in Theorem 4.18, condition (iii) in the Theorem is equivalent to the existence of  $g \in \tilde{S}_p^+$ ,  $R \in G_{D, \Lambda_1}$  such that  $D = \pi_g \cdot D$ ,  $L_2 = \pi_g \cdot L_1$ , and  $U_2 = U_1 R P_g^{-1}$ . But for all such  $R, \pi$ , we have  $R P_g^{-1} = R_0 P_{g_0}^{-1}$  for some  $R_0 \in G_{D, \Lambda_1}^0$  and  $g_0 \in \tilde{S}_p^+$  with  $\pi_{g_0} = \pi_g$ . Furthermore, for any  $\pi \in S_p$ , if  $\pi \cdot D = D$  then  $L_2 = \pi \cdot L_1 \iff \Lambda_2 = \pi \cdot \Lambda_1$ . Hence, under the hypotheses of Proposition 4.17, condition (iii) in Theorem 4.18 is equivalent to condition (ii) stated in the Proposition.

This establishes the “if and only if” statement in the Proposition. The final statement of the proposition follows from the fact that, in the notation of this proof, (4.18) is the equality  $A_2 = A_1$  (after multiplying both sides of (4.18) on the right by  $U^{-1}$ ), an equality that implies  $V_2 U_2^{-1} = \exp(A_2) = \exp(A_1) = V_1 U_1^{-1}$ . ■

## 5. Scaling-rotation distances for $\text{Sym}^+(3)$

For the case  $p = 3$ , we will obtain explicit formulas for all MSSR curves and scaling-rotation distances by using the quaternionic parametrization of  $SO(3)$ . In Section 6, we use this to give explicit descriptions of the set  $\mathcal{M}(X, Y)$  of MSSR curves between two points  $X, Y \in \text{Sym}^+(3)$  in all “nontrivial” cases.

### 5.1. Characterization of SR distance using quaternions

#### 5.1.1. Relation of quaternions to $SO(3)$

The space of  $\mathbf{H}$  of quaternions, with its usual real basis  $\{1, i, j, k\}$  identified with the standard basis of  $\mathbf{R}^4$ , and with  $\{i, j, k\}$  identified with the standard basis of

$\mathbf{R}^3$ , provides a convenient parametrization of  $SO(3)$ . Specifically, writing  $S_{\mathbf{H}}^3 = \{x_0 + x_1i + x_2j + x_3k : x_0^2 + x_1^2 + x_2^2 + x_3^2 = 1\}$ , there is a natural two-to-one Lie-group homomorphism  $\phi : S_{\mathbf{H}}^3 \rightarrow SO(3)$ , defined as follows. Using the basis  $\{i, j, k\}$  to identify  $\mathbf{R}^3$  with  $\text{Im}(\mathbf{H})$ , the space of purely imaginary quaternions, for  $q \in S_{\mathbf{H}}^3$  and  $x \in \text{Im}(\mathbf{H})$  we set  $\phi(q)(x) = qx\bar{q}$ , which lies in  $\text{Im}(\mathbf{H})$ . For  $q_1, q_2 \in S_{\mathbf{H}}^3$  we have  $\phi(q_2) = \phi(q_1)$  if and only if  $q_2 = \pm q_1$ . Thus, for any  $U \in SO(3)$ , if  $q_U \in \phi^{-1}(U)$  then

$$\phi^{-1}(U) = \{\pm q_U\}. \quad (5.1)$$

Let  $S_{\text{Im}(\mathbf{H})}^2 = \{\tilde{a} \in \text{Im}(\mathbf{H}) : \|\tilde{a}\| = 1\}$ . For  $\tilde{a} \in S_{\text{Im}(\mathbf{H})}^2$  and  $\theta \in [0, \pi]$  let  $R_{\theta, \tilde{a}}$  denotes counterclockwise rotation by angle  $\theta$  about the axis  $\tilde{a}$  (“counterclockwise” as determined by  $\tilde{a}$  using the right-hand rule). Let

$$SO(3)_{<\pi} := \{R_{\theta, \tilde{a}} : \tilde{a} \in S_{\text{Im}(\mathbf{H})}^2, \theta \in [0, \pi)\},$$

the set of non-involutions in  $SO(3)$ . The map  $s : SO(3)_{<\pi} \rightarrow S_{\mathbf{H}}^3$  defined by

$$s(R_{\theta, \tilde{a}}) = \cos \frac{\theta}{2} + (\sin \frac{\theta}{2})\tilde{a}. \quad (5.2)$$

is a smooth right-inverse to  $\phi$  on  $SO(3)_{<\pi}$  (i.e.  $\phi \circ s$  is the identity map on this domain), but  $s$  is not a homomorphism and cannot be extended continuously to all of  $SO(3)$ .

Distances between elements of  $SO(3)$  are related very simply to geodesic distances in  $S_{\mathbf{H}}^3$  with respect to the standard Riemannian metric on  $S^3 = S_{\mathbf{H}}^3$ . For  $U, V \in SO(3)$ ,

$$\begin{aligned} d_{SO(3)}(U, V) &= 2 \min\{d_{S^3}(r_U, r_V) : r_U \in \phi^{-1}(U), r_V \in \phi^{-1}(V)\} \\ &= 2 \cos^{-1} |\text{Re}(\overline{r_U} r_V)| \text{ where } r_U, r_V \text{ are as in previous line.} \end{aligned}$$

Alternatively,  $d_{SO(3)}(U, V) = d_{SO(3)}(I, U^{-1}V) = 2 \cos^{-1} |\text{Re}(q_{U^{-1}V})|$ , where  $q_{U^{-1}V}$  is either of the two elements of  $\phi^{-1}(U^{-1}V)$ . Thus

$$d_{SO(3)}(U, V) = 2 \cos^{-1} |\text{Re}(\overline{q_U} q_V)| = 2 \cos^{-1} |\text{Re}(q_{U^{-1}V})| \quad (5.3)$$

where each of  $q_U, q_V, q_{U^{-1}V}$  is either of the two elements in  $S^3$  mapped by  $\phi$  to  $U, V$ , and  $U^{-1}V$  respectively.

### 5.1.2. Quaternionic pre-images of signed permutation matrices

For every subgroup  $H \subset SO(3)$ , let  $\hat{H}$  denote the pre-image  $\phi^{-1}(H) \subset S_{\mathbf{H}}^3$ . Writing  $\Gamma := \hat{S}_3^+ \subset SO(3)$ , the 24-element group of even signed permutation matrices, the 48 elements of  $\hat{\Gamma}$  are the following:

$$\pm 1, \pm i, \pm j, \pm k, \quad (5.4)$$

$$\frac{1}{\sqrt{2}}(\pm e_m \pm e_n), \text{ where } e_0 = 1, e_2 = i, e_3 = j, e_4 = k, \text{ and } m < n, \quad (5.5)$$

$$\frac{1}{2}(\pm 1 \pm i \pm j \pm k) \quad (5.6)$$

(all sign-combinations allowed in all sums). Under  $\phi$ , the eight elements (5.4) are mapped to the four even sign-change matrices, the 24 elements (5.5) are mapped to the 12 positive-determinant “signed transposition matrices” (permutation-matrices corresponding to transpositions, with an odd number of 1’s replaced by  $-1$ ’s), and the 16 elements (5.6) are mapped to the 8 positive-determinant “signed cyclic-permutation matrices” (permutation-matrices corresponding to cyclic permutations, with an even number of 1’s replaced by  $-1$ ’s).

### 5.1.3. Parameters corresponding to different strata

For any subgroups  $H_1, H_2$  of  $SO(3)$ , the map  $\phi$  induces a bijection  $\widehat{H_1} \backslash \widehat{\Gamma} / \widehat{H_2} \rightarrow H_1 \backslash \Gamma / H_2$ . Thus if  $\tilde{Z}$  is a set of representatives of  $\widehat{\Gamma_D^0} \backslash \widehat{\Gamma} / \widehat{\Gamma_\Lambda^0}$  in  $\widehat{\Gamma}$ , then  $\phi(\tilde{Z})$  is a set  $Z$  of representatives of  $\Gamma_D^0 \backslash \Gamma / \Gamma_\Lambda^0$  in  $\Gamma$ .

Now let  $X, Y, (U, D)$ , and  $(V, \Lambda)$  be as in Proposition 4.9, and let  $\tilde{Z}$  be a set of representatives of  $\widehat{\Gamma_D^0} \backslash \widehat{\Gamma} / \widehat{\Gamma_\Lambda^0}$ . For  $\zeta \in \widehat{\Gamma}$ , define  $\pi_\zeta = \pi_{\phi(\zeta)} \in S_3$  (see Definition 2.14).

From equation (5.3) and the fact that  $\phi$  is a homomorphism, it follows that in the setting of equation (4.13) (with  $p = 3$ ), for all  $r_U \in \phi^{-1}(R_U), r_V \in \phi^{-1}(R_V), g \in \tilde{S}_3^+$ , and  $\zeta_g \in \phi^{-1}(g)$ ,

$$d_{SO(3)}(UR_U, VR_V P_g^{-1})^2 = 4 \left( \cos^{-1} \left| \operatorname{Re} \left( r_V \overline{\zeta_g} \overline{r_U} q_{U^{-1}V} \right) \right| \right)^2. \quad (5.7)$$

From Proposition 4.9, we therefore have

$$\begin{aligned} d_{\mathcal{SR}}(X, Y)^2 = & \min_{\zeta \in \tilde{Z}} \left\{ 4k \left( \min \left\{ \cos^{-1} \left| \operatorname{Re} \left( r_V \overline{\zeta} \overline{r_U} q_{U^{-1}V} \right) \right| : r_U \in \widehat{G_D^0}, r_V \in \widehat{G_\Lambda^0} \right\} \right)^2 \right. \\ & \left. + \left\| \log(\Lambda_{\pi_\zeta} D^{-1}) \right\|^2 \right\}. \end{aligned} \quad (5.8)$$

As equation (5.8) suggests, computing  $d_{\mathcal{SR}}(X, Y)$  is a minimization problem that breaks into two parts, one over the discrete parameter-set  $\tilde{Z}$  and the other over the (potentially) “continuous” parameter-set  $\widehat{G_D^0} \times \widehat{G_\Lambda^0}$ . Both parameter-sets depend on  $X$  and  $Y$ . For each  $\zeta \in \tilde{Z}$ , the inner minimum over  $\widehat{G_D^0} \times \widehat{G_\Lambda^0}$  on the first line of (5.8) is computed, then added to the term on the second line.

If  $X$  or  $Y$  lies in the bottom stratum of  $\operatorname{Sym}^+(p)$  (i.e., has only one distinct eigenvalue), then the set  $\tilde{Z}$  has only one element  $\zeta$ , which we can take to be  $1 \in \mathbf{H}$ , and at least one of the groups  $\widehat{G_D^0}, \widehat{G_\Lambda^0}$  is all of  $S_{\mathbf{H}}^3$ . The set  $\{r_V \overline{\zeta} \overline{r_U} : (r_U, r_V) \in \widehat{G_D^0} \times \widehat{G_\Lambda^0}\}$  is simply  $S_{\mathbf{H}}^3$ , the inner minimum in (5.8) is 0, and we immediately obtain  $d_{\mathcal{SR}}(X, Y) = \|\log(\Lambda D^{-1})\|$ . We do not need to use quaternions to obtain this result; it follows just as quickly from (4.13).

At the other extreme, if  $X$  and  $Y$  both lie in the top stratum of  $\operatorname{Sym}^+(p)$  (i.e. both have three distinct eigenvalues) then  $\widehat{G_D^0} = \widehat{G_\Lambda^0} = \{\pm 1\}$ , and the

inner minimum is trivial to compute (the argument of the arc-cosine term is independent of  $(r_U, r_V)$ ), so we are reduced immediately to a single minimization over  $\tilde{Z}$ . As in the previous case, we do not need the quaternionic reframing of the distance formula at all: already in (4.12) we have  $G_D^0 = G_\Lambda^0 = \{I\}$ , so the distance can be found simply by minimizing over the discrete variable  $g \in Z = \tilde{S}_3^+$ . We need only have a computer calculate  $d_M((U, D), (VP_g^{-1}, g \cdot \Lambda))$  for each of the 24  $g$ 's and return the corresponding minimal pairs and MSSR curves. For combinatorial reasons, a complete algebraic classification of the pairs  $(X, Y)$  (with  $X, Y$  both in the top stratum of  $\text{Sym}^+(3)$ ) for which  $\mathcal{M}(X, Y)$  has a given cardinality would be very complex, and we do not attempt this. However, in the online supplement, we use quaternions to help understand analytically the possibilities as  $X$  and  $Y$  vary, and provide several illustrative examples.

For the above reasons, for the remainder of this section we focus on the cases in which  $X$  and  $Y$  do not both lie in the top stratum of  $\text{Sym}^+(3)$ , and neither lies in the bottom stratum. Thus we restrict attention to the cases in which one of the matrices  $X, Y$  has exactly two distinct eigenvalues, and the other has either two or three. We refer to these cases as the “nontrivial” cases (because the set of distances between elements of  $\mathcal{E}_X$  and elements of  $\mathcal{E}_Y$  is not a finite set). To analyze them we introduce the following notation:

$$\begin{aligned} \mathcal{S}_{\text{top}} &:= \mathcal{S}_{1+1+1} \subset \text{Sym}^+(3), \\ \mathcal{S}_{\text{mid}} &:= \mathcal{S}_{2+1} \\ &= \{X \in \text{Sym}^+(3) : X \text{ has exactly 2 distinct eigenvalues}\} \\ &\quad \subset \text{Sym}^+(3), \\ \mathcal{D}_{J_1} &:= \mathcal{D}_{\{\{1\}, \{2,3\}\}} \\ &= \{\text{diag}(d_1, d_2, d_2) : d_1, d_2 > 0, d_1 \neq d_2\} \subset \text{Diag}^+(3). \end{aligned}$$

## 5.2. Scaling-rotation distances for $\text{Sym}^+(3)$ in the nontrivial cases

From now till the end of Section 6 we assume that  $X \in \mathcal{S}_{\text{mid}}$  and that either  $Y \in \mathcal{S}_{\text{top}}$  or  $Y \in \mathcal{S}_{\text{mid}}$ . Then  $X$  has an eigen-decomposition  $(U, D)$  with  $D \in \mathcal{D}_{J_1}$ , and if  $Y \in \mathcal{S}_{\text{mid}}$  then  $Y$  has a eigen-decomposition  $(V, \Lambda)$  with  $\Lambda \in \mathcal{D}_{J_1}$ . We will always assume that our pairs  $(U, D), (V, \Lambda)$  have been chosen this way. Then we have

$$G_D^0 = G_{\mathcal{D}_{J_1}}^0 := \left\{ \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & R \end{bmatrix} : R \in SO(2) \right\}, \quad G_\Lambda^0 = \begin{cases} \{I\} & \text{if } Y \in \mathcal{S}_{\text{top}}, \\ G_{\mathcal{D}_{J_1}}^0 & \text{if } Y \in \mathcal{S}_{\text{mid}}. \end{cases}$$

It is not hard to check that

$$\widehat{G_D^0} = S_{\mathbf{C}}^1 := \{\exp(ti) : t \in \mathbf{R}\} \subset \mathbf{C} \subset \mathbf{H}, \quad (5.9)$$

$$\widehat{G_\Lambda^0} = \begin{cases} \{\pm 1\} & \text{if } Y \in \mathcal{S}_{\text{top}}, \\ S_{\mathbf{C}}^1 & \text{if } Y \in \mathcal{S}_{\text{mid}}. \end{cases} \quad (5.10)$$

The inner minimum in (5.8) is then

$$\min_{r_U \in S_{\mathbb{C}}^1} \left\{ \cos^{-1} \left| \operatorname{Re} \left( \bar{\zeta} \overline{r_U} q_{U^{-1}V} \right) \right| \right\} \quad \text{if } Y \in \mathcal{S}_{\text{top}}, \quad (5.11)$$

$$\min_{r_U, r_V \in S_{\mathbb{C}}^1} \left\{ \cos^{-1} \left| \operatorname{Re} \left( r_V \bar{\zeta} \overline{r_U} q_{U^{-1}V} \right) \right| \right\} \quad \text{if } Y \in \mathcal{S}_{\text{mid}}. \quad (5.12)$$

Obviously, minimizing the arc-cosines above is equivalent to maximizing

$$\left| \operatorname{Re} \left( \bar{\zeta} \overline{r_U} q_{U^{-1}V} \right) \right| \quad \text{if } Y \in \mathcal{S}_{\text{top}}, \quad (5.13)$$

$$\left| \operatorname{Re} \left( r_V \bar{\zeta} \overline{r_U} q_{U^{-1}V} \right) \right| \quad \text{if } Y \in \mathcal{S}_{\text{mid}}, \quad (5.14)$$

where the maximum is taken over  $(r_U, r_V) \in S_{\mathbb{C}}^1 \times S_{\mathbb{C}}^1$  in (5.14), and over just  $r_U \in S_{\mathbb{C}}^1$  in (5.13).

### 5.2.1. The discrete parameter-sets $\tilde{Z}$ in the nontrivial cases

To compute the outer minimum (over  $\zeta$ ) in (5.8), we will need to select sets  $\tilde{Z}$  of representatives of  $\widehat{\Gamma_D^0} \backslash \widehat{\Gamma} / \widehat{\Gamma_\Lambda^0}$  in two cases: (i)  $J_D = J_1 := \{1, \{2, 3\}\}$ ,  $J_\Lambda = J_{\text{top}} := \{\{1\}, \{2\}, \{3\}\}$ , and (ii)  $J_D = J_1 = J_\Lambda$ . Let us write  $\Gamma_1 := \Gamma_{J_1}^0$ . For case (i), since  $\widehat{\Gamma_{J_{\text{top}}}^0} = \{\pm 1\}$ , which commutes with every element of  $\widehat{\Gamma}$  and is a subgroup of  $\widehat{\Gamma_J^0}$  for every  $J$ , the double-coset space  $\widehat{\Gamma_1} \backslash \widehat{\Gamma} / \widehat{\Gamma_{J_{\text{top}}}^0}$  is simply the set  $\widehat{\Gamma_1} \backslash \widehat{\Gamma}$  of right  $\widehat{\Gamma_1}$ -cosets in  $\widehat{\Gamma}$ . Observe that  $\widehat{\Gamma_1} = \widehat{G_{J_1}^0} \cap \widehat{\Gamma} = S_{\mathbb{C}}^1 \cap \widehat{\Gamma} = \{\pm 1, \pm i, \frac{\pm 1 \pm i}{\sqrt{2}}\} = \{e^{2n\pi i/8} : n = 0, 1, \dots, 7\}$ . Thus the cardinality of  $\widehat{\Gamma_1} \backslash \widehat{\Gamma}$  is  $48/8 = 6$ . One can check that the following set  $\tilde{Z}_{1,*}$  contains a representative of each of the six right  $\widehat{\Gamma_1}$ -cosets:

$$\tilde{Z}_{1,*} := \left\{ 1, j, \frac{1 \pm j}{\sqrt{2}}, \frac{1 \pm k}{\sqrt{2}} \right\}. \quad (5.15)$$

For case (ii), the double-coset space can be viewed as the set of orbits under the action of  $\widehat{\Gamma_1}$  on  $\widehat{\Gamma_1} \backslash \widehat{\Gamma}$  (the coset-space in case (i)) by right-multiplication. Thus a set of representatives can be found by imposing the double-coset equivalence relation on the set  $\tilde{Z}_{1,*}$  above. The four elements  $\frac{1 \pm j}{\sqrt{2}}, \frac{1 \pm k}{\sqrt{2}}$  all lie in the same  $\widehat{\Gamma_1}$  double-coset, since

$$-i \frac{1+j}{\sqrt{2}} i = \frac{1-j}{\sqrt{2}}, \quad -i \frac{1+k}{\sqrt{2}} i = \frac{1-k}{\sqrt{2}}, \quad \text{and} \quad \frac{1+i}{\sqrt{2}} \frac{1+j}{\sqrt{2}} \frac{1-i}{\sqrt{2}} = \frac{1+k}{\sqrt{2}}.$$

It is easily checked that no two of  $1, j$ , and  $\frac{1 \pm j}{\sqrt{2}}$  lie in the same  $(\widehat{\Gamma_1}, \widehat{\Gamma_1})$  double-coset. Hence  $Z_{1,1} := \{1, j, \frac{1 \pm j}{\sqrt{2}}\}$  is a set of representatives of  $\widehat{\Gamma_1} \backslash \widehat{\Gamma} / \widehat{\Gamma_1}$ .

The elements  $\zeta$  of  $Z_{1,*}$  are listed in Table 2, along with the images  $\phi(\zeta) \in SO(3)$  and  $\pi_\zeta \in S_3$ . Since  $Z_{1,1} \subset Z_{1,*}$ , a separate listing for  $Z_{1,1}$  is not needed.

$\zeta \in \tilde{Z}_{1,*}$	1	$j$	$\zeta_{j,\epsilon} := \frac{1+\epsilon j}{\sqrt{2}}, \epsilon \in \{\pm 1\}$	$\zeta_{k,\epsilon} := \frac{1+\epsilon k}{\sqrt{2}}, \epsilon \in \{\pm 1\}$
$\phi(\zeta) \in Z_{1,*}$	$I$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -\epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$\pi_\zeta \in S_3$	$\pi_{\text{id}}$	$\pi_{\text{id}}$	$\pi_{13}$	$\pi_{12}$

TABLE 2

Representatives of the double-coset space  $\widehat{\Gamma_1} \backslash \widehat{\Gamma} / \widehat{\Gamma_{\text{J}_{\text{top}}^0}} = \widehat{\Gamma_1} \backslash \widehat{\Gamma}$ , where  $\widehat{\Gamma_1} = \widehat{\Gamma_{\text{J}_1^0}^0}$ . A set of representatives of  $\widehat{\Gamma_1} \backslash \widehat{\Gamma} / \widehat{\Gamma_1}$  is  $\tilde{Z}_{1,1} := \{1, j, \zeta_{j,+}\}$ .

In Table 2 and henceforth, we write  $\pi_{\text{id}}$  for the identity permutation, and, for distinct  $a, b \in \{1, 2, 3\}$ , we write  $\pi_{ab}$  for the transposition  $(ab)$ , the permutation that just interchanges  $a$  and  $b$ .

**Remark 5.1** As seen in Section 3.3.2,  $\mathcal{E}_X$  has six connected components, each diffeomorphic to the circle  $G_{\text{J}_1}^0$ . In Proposition 2.19, for general  $p$  and  $X$ , we exhibited a bijection between  $\text{Comp}(\mathcal{E}_X)$  and the left-coset space  $\tilde{S}_p^+ / \Gamma_{\text{J}_D}^0$ . For any group  $G$  and subgroup  $H$ , the inversion map  $G \rightarrow G$  induces a 1-1 correspondence between left  $H$ -cosets and right  $H$ -cosets, so (for general  $p$  and  $X$ ),  $\text{Comp}(\mathcal{E}_X)$  is also in bijection with  $\Gamma_{\text{J}_D}^0 \backslash \tilde{S}_p^+$ . In our current  $p = 3, X \in \mathcal{S}_{\text{mid}}$  setting, the set  $Z_{1,*} := \{\phi(\zeta) : \zeta \in \tilde{Z}_{1,*}\}$ , is a set of representatives of  $\Gamma_1 \backslash \tilde{S}_3^+ / \Gamma_{\text{J}_{\text{top}}} = \Gamma_1 \backslash \tilde{S}_3^+$ . The fact that right  $\Gamma_1$ -cosets appear here instead of left cosets is an artifact of our having chosen  $X$ , rather than  $Y$ , to lie in  $\mathcal{S}_{\text{mid}}$ .

### 5.2.2. Hypercomplex reformulation of the continuous-parameter minimization problem

We now have

$$d_{\mathcal{SR}}(X, Y)^2 = d(\mathcal{E}_X, \mathcal{E}_Y)^2 = \begin{cases} \min_{\zeta \in \tilde{Z}_{1,*}} \left\{ 4k \left( \min_{r_U \in S_{\mathbf{C}}^1} \{ \cos^{-1} |\text{Re}(\bar{\zeta} \overline{r_U} q_{U^{-1}V})| \} \right)^2 + \|\log(\Lambda_{\pi_\zeta} D^{-1})\|^2 \right\} \\ \text{if } Y \in \mathcal{S}_{\text{top}}, \\ \min_{\zeta \in \tilde{Z}_{1,1}} \left\{ 4k \left( \min_{r_U, r_V \in S_{\mathbf{C}}^1} \{ \cos^{-1} |\text{Re}(r_V \bar{\zeta} \overline{r_U} q_{U^{-1}V})| \} \right)^2 + \|\log(\Lambda_{\pi_\zeta} D^{-1})\|^2 \right\} \\ \text{if } Y \in \mathcal{S}_{\text{mid}}. \end{cases} \quad (5.16)$$

To allow us to refer efficiently to the minimization-parameters in (5.16) without too much separate notation for the two cases  $Y \in \mathcal{S}_{\text{top}}, Y \in \mathcal{S}_{\text{mid}}$ , for both cases we will refer to the triple  $(\zeta, r_U, r_V)$ , with the understanding that we always take  $r_V = 1$  when  $Y \in \mathcal{S}_{\text{top}}$ .

Recall that quaternions can be written in “hypercomplex” form: we regard the complex numbers  $\mathbf{C}$  as the subset  $\{a + bi\} \subset \mathbf{H}$ , and write  $x_0 + x_1 i + x_2 j + x_3 k =$

$z + wj = z + j\bar{w}$ , where  $z = x_0 + x_1i, w = x_2 + x_3i$ . This gives us a natural identification

$$S_{\mathbf{H}}^3 \longleftrightarrow S_{\mathbf{C}^2}^3 := \{(z, w) \in \mathbf{C}^2 : |z|^2 + |w|^2 = 1\}. \quad (5.17)$$

To perform the maximization of (5.14) and (5.13) (in order to minimize the arc-cosines in (5.11) and (5.12)), we will write  $q_{U^{-1}V}$  in hypercomplex form:

$$q_{U^{-1}V} = z + wj, \quad (z, w) \in S_{\mathbf{C}^2}^3. \quad (5.18)$$

Henceforth whenever we refer to the quantities  $z$  and  $w$ , they are regarded as functions of the pair  $(U, V)$ , satisfying (5.18), and with the pair  $(z, w)$  determined only up to an overall sign.

Because the parameters  $r_U, r_V$  in (5.14) and (5.13) run over the unit circle in  $\mathbf{C}$ , it is easy to maximize (5.14) and (5.13) explicitly for each  $\zeta$  in  $\tilde{Z}_{1,*}$  and  $\tilde{Z}_{1,1}$ , respectively, and then to maximize over  $\zeta$ . To express some of our answers, we define the following quantities, which we may regard as functions of the pair  $(U, V)$ :

$$\varphi := \cos^{-1}(\max\{|z|, |w|\}), \quad (5.19)$$

$$\beta := \cos^{-1} \sqrt{\frac{1 + 2|\operatorname{Re}(\bar{z}w)|}{2}}, \quad \beta' := \cos^{-1} \sqrt{\frac{1 + 2|\operatorname{Im}(\bar{z}w)|}{2}}. \quad (5.20)$$

Note that  $\varphi, \beta$ , and  $\beta'$  all lie in the interval  $[0, \frac{\pi}{4}]$ .

**Remark 5.2** Let  $(U, D) \in \mathcal{E}_X, (V, \Lambda) \in \mathcal{E}_Y$  be eigen-decompositions of  $X, Y$  respectively. When  $X$  and  $Y$  both lie in  $\mathcal{S}_{\text{mid}}$ , the ellipsoids corresponding to the matrices  $X$  and  $Y$  are surfaces of revolution. When  $D$  and  $\Lambda$  both lie in  $\mathcal{D}_{J_1}$ , the case in which

$$w = 0 \text{ or } z = 0 \quad (5.21)$$

in (5.18) has a simple geometric interpretation, and will have special significance later in Theorem 6.4. Observe that  $w = 0$  if and only if  $V = UR$  for some  $R \in G_{\mathcal{D}_{J_1}}^0$ , while  $z = 0$  if and only if  $V = UR$  for some  $R \in G_{\mathcal{D}_{J_1}}^0 j := \{R\phi(j) : R \in G_{\mathcal{D}_{J_1}}^0\}$ . But  $G_{\mathcal{D}_{J_1}}^0$  and  $G_{\mathcal{D}_{J_1}}^0 j$  are exactly the two connected components of  $G_{\mathcal{D}_{J_1}}$ . Hence (5.21) is equivalent to  $V = UR$  for some  $R \in G_{\mathcal{D}_{J_1}}$ , which in turn is equivalent to  $V\Lambda V' = U\Lambda U^{-1}$ . Thus (when  $D, \Lambda \in \mathcal{D}_{J_1}$ ) the following are all equivalent: (i)  $\varphi = 0$ ; (ii)  $w = 0$  or  $z = 0$ ; (iii) simultaneously,

$$X = UDU^{-1} \text{ and } Y = U\Lambda U^{-1}; \quad (5.22)$$

(iv) the ellipsoids of revolution corresponding to the matrices  $X$  and  $Y$  have the same axis of symmetry. The latter condition is obviously intrinsic to the pair  $(X, Y)$ , independent of any choices of eigen-decompositions. Note also that when we want to find all minimal smooth scaling-rotation curves from  $X$  to  $Y$ , we do not need to express these in terms of *arbitrary* eigen-decompositions with  $D, \Lambda \in \mathcal{D}_{J_1}$ ; it suffices to use any that we find convenient. Thus, given the eigen-decomposition  $(U, D)$  of  $X$ , if (5.21) (hence (5.22)) holds we are free to replace  $V$  with  $U$ , in which case  $U^{-1}V = I$  and  $(z, w) = (\pm 1, 0)$ . We will adopt the following convention:



**Convention 5.3.** If  $D, \Lambda \in \mathcal{D}_{J_1}$  and  $U, V$  are such that  $w = 0$  or  $z = 0$ , we replace  $V$  with  $U$ , and replace  $(z, w)$  with  $(1, 0)$ . We do not change  $U$ .

### 5.2.3. Closed-form formulas for $\text{Sym}^+(3)$ distances

**Theorem 5.4** Let  $X, Y \in \text{Sym}^+(3)$ ,  $(U, D) \in \mathcal{E}_X$ , and  $(V, \Lambda) \in \mathcal{E}_Y$ . If  $X \in \mathcal{S}_{\text{mid}}$  assume  $D \in \mathcal{D}_{J_1}$ ; if  $Y \in \mathcal{S}_{\text{mid}}$  assume  $\Lambda \in \mathcal{D}_{J_1}$ . The distance  $d_{\mathcal{SR}}(X, Y)$  is given as follows.

(i) If  $X, Y \in \mathcal{S}_{\text{top}}$ , then

$$d_{\mathcal{SR}}(X, Y)^2 = \min_{g \in \mathcal{S}_3^+} \left\{ \frac{k}{2} \|\log(U^{-1}VP_g^{-1})\|^2 + \|\log(D^{-1}(\pi_g \cdot \Lambda))\|^2 \right\}.$$

(ii) If  $X \in \mathcal{S}_{\text{mid}}, Y \in \mathcal{S}_{\text{top}}$ , then

$$d_{\mathcal{SR}}(X, Y) = \min \{ \ell_{\text{id}}, \ell_{(13)}, \ell_{(12)} \}, \quad (5.23)$$

where

$$\ell_{\text{id}} = \sqrt{4k\varphi^2 + \|\log(\Lambda D^{-1})\|^2}, \quad (5.24)$$

$$\ell_{(13)} = \sqrt{4k\beta^2 + \|\log(\Lambda_{\pi_{13}} D^{-1})\|^2}, \quad (5.25)$$

$$\ell_{(12)} = \sqrt{4k(\beta')^2 + \|\log(\Lambda_{\pi_{12}} D^{-1})\|^2}, \quad (5.26)$$

and where  $\phi, \beta, \beta' \in [0, \frac{\pi}{4}]$  are defined by (5.18) and (5.19)–(5.20). Writing  $D$  as  $\text{diag}(d_1, d_2, d_2)$  and  $\Lambda$  as  $\text{diag}(\lambda_1, \lambda_2, \lambda_3)$ , we also have the following comparisons of  $\ell_{\text{id}}, \ell_{(13)}$ , and  $\ell_{(12)}$ :

$$\ell_{\text{id}}^2 - \ell_{(13)}^2 = 4k(\varphi^2 - \beta^2) - 2 \log\left(\frac{d_1}{d_2}\right) \log\left(\frac{\lambda_1}{\lambda_3}\right), \quad (5.27)$$

$$\ell_{\text{id}}^2 - \ell_{(12)}^2 = 4k(\varphi^2 - (\beta')^2) - 2 \log\left(\frac{d_1}{d_2}\right) \log\left(\frac{\lambda_1}{\lambda_2}\right), \quad (5.28)$$

$$\ell_{(13)}^2 - \ell_{(12)}^2 = 4k(\beta^2 - (\beta')^2) + 2 \log\left(\frac{d_1}{d_2}\right) \log\left(\frac{\lambda_2}{\lambda_3}\right). \quad (5.29)$$

(iii) If  $X, Y$  both lie in  $\mathcal{S}_{\text{mid}}$ , then

$$d_{\mathcal{SR}}(X, Y) = \min \{ \ell_{\text{id}}, \ell_{(13)} \}, \quad (5.30)$$

where

$$\ell_{\text{id}} = \sqrt{4k\varphi^2 + \|\log(\Lambda D^{-1})\|^2}, \quad (5.31)$$

$$\ell_{(13)} = \sqrt{4k\left(\frac{\pi}{4} - \varphi\right)^2 + \|\log(\Lambda_{\pi_{13}} D^{-1})\|^2}. \quad (5.32)$$

Writing  $D$  as  $\text{diag}(d_1, d_2, d_2)$  and  $\Lambda$  as  $\text{diag}(\lambda_1, \lambda_2, \lambda_2)$ , we also have the following comparison of  $\ell_{\text{id}}$  and  $\ell_{(13)}$ :

$$\ell_{\text{id}}^2 - \ell_{(13)}^2 = 2k\pi(\varphi - \frac{\pi}{8}) - 2\log\left(\frac{d_1}{d_2}\right)\log\left(\frac{\lambda_1}{\lambda_2}\right). \quad (5.33)$$

(iv) If  $X \in \mathcal{S}_{\text{bot}} := \mathcal{S}_{J_{\text{bot}}}$  then  $d_{\mathcal{SR}}(X, Y) = d_{\mathcal{D}^+}(D, \Lambda) = \|\log(D^{-1}\Lambda)\|$ , regardless of which stratum  $Y$  lies in.

**Proof:**

(i) Since  $G_D^0 = G_\Lambda^0 = \{I\}$  in this case, (5.23) follows immediately from (4.13) in Proposition 4.9.

(ii) From the discussion in Section 4,  $d_{\mathcal{SR}}(X, Y)$  is given by (5.16). We proceed by determining the “inner” minimum for each  $\zeta \in \tilde{Z}_{1,*}$ , and comparing the answers for the different  $\zeta$ 's. As noted in Section 4, for a given  $\zeta$ , minimizing the arc-cosine in (5.16) is equivalent to maximizing expression (5.13). Below, we use the notation (5.18), and for any nonzero  $\xi \in \mathbf{C}$  we set  $\hat{\xi} := \xi/|\xi|$ . Facts used repeatedly in these calculations are that for all  $\xi \in \mathbf{C}$ , (i)  $\xi j$  and  $\xi k$  are linear combinations of  $j$  and  $k$  with real coefficients, hence are purely imaginary; and (ii)  $j\xi = \bar{\xi}j$  and  $k\xi = \bar{\xi}k$ . Using these facts, we compute

$$f_1(\zeta, r_U) := \text{Re}(\bar{r}_U(z + wj)) = \begin{cases} \text{Re}(\bar{r}_U z) & \text{if } \zeta = 1, \\ \text{Re}(\bar{r}_U w) & \text{if } \zeta = j, \\ \frac{1}{\sqrt{2}}\text{Re}(\bar{r}_U(z + \epsilon w)) & \text{if } \zeta = \zeta_{j,\epsilon}, \\ \frac{1}{\sqrt{2}}\text{Re}(\bar{r}_U(z - \epsilon iw)) & \text{if } \zeta = \zeta_{k,\epsilon}. \end{cases} \quad (5.34)$$

Hence for each  $\zeta \in \tilde{Z}_{1,*}$ , the value of  $\max_{r_U \in S_{\mathbf{C}}^1} |\text{Re}(\bar{\zeta} \bar{r}_U(z + jw))|$  is the entry in the last column of the corresponding line of Table 3; let us denote this as  $|f_2(\zeta)|$ , where  $f_2(\zeta) \in \mathbf{C}$ . The set of elements  $r_U \in S_{\mathbf{C}}^1$  at which the maximum is attained is  $\{\pm \widehat{f_2(\zeta)}\}$  if  $f_2(\zeta) \neq 0$ , and all of  $S_{\mathbf{C}}^1$  if  $f_2(\zeta) = 0$ .

Since  $|z|^2 + |w|^2 = 1$ , we have  $|z \pm w|^2 = 1 \pm 2\text{Re}(\bar{z}w)$ ,  $|z \pm iw|^2 = 1 \mp 2\text{Im}(\bar{z}w)$ . Thus, grouping together the elements  $\zeta \in \tilde{Z}_{1,*}$  corresponding to the same permutation  $\pi_\zeta$ , we have the following:

$$|f_2(\zeta)| = \max_{r_U \in S_{\mathbf{C}}^1} |\text{Re}(\bar{\zeta} \bar{r}_U(z + jw))| = \begin{cases} \max\{|z|, |w|\} & \text{if } \pi_\zeta = \pi_{\text{id}}, \\ \sqrt{\frac{1+2|\text{Re}(\bar{z}w)|}{2}} & \text{if } \pi_\zeta = \pi_{13}, \\ \sqrt{\frac{1+2|\text{Im}(\bar{z}w)|}{2}} & \text{if } \pi_\zeta = \pi_{12} \end{cases} \quad (5.35)$$

(assuming  $\zeta \in \tilde{Z}_{1,*}$ ). Equation (5.23) now follows from the definitions (5.19)–(5.20) and equations (5.35) and (5.16).

Now let  $a = \log d_1, b = \log d_2, c = \log \lambda_1, d = \log \lambda_2, f = \log \lambda_3$ . An easy calculation yields  $\|\log(\Lambda D^{-1})\|^2 - \|\log((\pi_{13}\Lambda)D^{-1})\|^2 = -2(a-b)(c-f)$ , from which equation (5.27) follows. The derivations of (5.28) and (5.29) are similar.

(iii) We use the same strategy as in part (ii), but now with  $\zeta$  ranging only over the set  $\tilde{Z}_{1,1} = \{1, j, \zeta_{j,+}\}$ , and with  $r_U, r_V$  both allowed to vary over  $S_{\mathbb{C}}^1$ . This time we find

$$f_3(\zeta, r_U, r_V) := \operatorname{Re}(r_V \bar{\zeta} \bar{r}_U (z + wj)) = \begin{cases} \operatorname{Re}(r_V \bar{r}_U z) & \text{if } \zeta = 1, \\ \operatorname{Re}(r_V r_U \bar{w}) & \text{if } \zeta = j, \\ \frac{1}{\sqrt{2}} \operatorname{Re}(r_V [\bar{r}_U z + r_U \bar{w}]) & \text{if } \zeta = \zeta_{j,+} . \end{cases} \quad (5.36)$$

It is obvious from (5.36) that

$$|f_4(\zeta)| := \max_{r_U, r_V \in S_{\mathbb{C}}^1} |\operatorname{Re}(r_V \bar{\zeta} \bar{r}_U (z + wj))| = \begin{cases} |z| & \text{if } \zeta = 1, \\ |w| & \text{if } \zeta = j, \end{cases} \quad (5.37)$$

and that the pairs  $(r_U, r_V)$  at which the maximum is achieved are all those for which  $r_V \bar{r}_U = \bar{z}$  if  $\zeta = 1$ , and for which  $r_V r_U = \pm \hat{w}$  if  $\zeta = j$ . Thus, for these two  $\zeta$ 's, the set of maximizing pairs  $(r_U, r_V)$  is the two circles' worth of pairs appearing in the triples  $(\zeta, r_U, r_V)$  in the lines for classes  $A'_1$  and  $A'_2$  in Table 3, and the last entry of each line is the corresponding maximum value (5.37).

Now consider  $\zeta = \zeta_{j,+} = \frac{1+j}{\sqrt{2}}$ . Since  $r_U, r_V$  are unit complex numbers, it is clear from (5.36) that

$$|f_3(\zeta_{j,+}, r_U, r_V)| \leq |\operatorname{Re}(r_V \bar{\zeta} \bar{r}_U (z + wj))| \leq \frac{|z| + |w|}{\sqrt{2}} \quad (5.38)$$

for all  $r_U, r_V$ .

First assume that  $z \neq 0 \neq w$ . Then the upper bound on  $|f_3(\zeta_{j,+}, r_U, r_V)|$  in (5.38) will be achieved by a pair  $(r_U, r_V)$  if and only if

$$(r_V \bar{r}_U, r_V r_U) = \pm(\bar{z}, \hat{w}) . \quad (5.39)$$

But (5.39) is easily solved; the solution-set is exactly the set of four pairs  $(\pm(\hat{w}\hat{z})^{1/2}, \pm(\hat{w}\hat{z})^{1/2})$  appearing Table 3 for Class B'. Thus the upper bound in (5.38) is actually the maximum value of  $|f_3(\zeta_{j,+}, \cdot, \cdot)|$ .

Now assume that  $w = 0$  or  $z = 0$ ; we define the corresponding set of pairs in  $\mathcal{E}_X \times \mathcal{E}_Y$  (i.e. those pairs  $((U\phi(r_U), D), (V\phi(r_V)\phi(\zeta_{j,+})', \Lambda_{\pi_{\zeta_{j,+}}}))$  for which  $(r_U, r_V)$  maximizes  $|f_3(\zeta_{j,+}, \cdot, \cdot)|$ ) to be Class C'. If  $w = 0$  then  $|z| = 1$ , and we need only maximize  $\frac{1}{\sqrt{2}}|\operatorname{Re}(r_V \bar{r}_U z)|$ . Since  $|z| = 1$ , the maximum value is  $\frac{1}{\sqrt{2}}$ , and is achieved at all pairs  $(r_U, r_V)$  for which  $r_V \bar{r}_U = \pm \bar{z}$ . Similarly, if  $z = 0$  then  $|w| = 1$ , and we need only maximize  $\frac{1}{\sqrt{2}}|\operatorname{Re}(r_V r_U \bar{w})|$ . The maximum is again  $\frac{1}{\sqrt{2}}$ , now achieved at all pairs  $(r_U, r_V)$  for which  $r_V r_U = \pm w$ .

Hence, for  $\zeta = \zeta_{j,+}$ , whether or not  $z$  and  $w$  are both nonzero, the right-hand side of (5.38) is the maximum value of  $|f_3(\zeta_{j,+}, \cdot, \cdot)|$ . But if  $z \neq 0 \neq w$  there are only four maximizing pairs  $(r_U, r_V)$ , while if  $w = 0$  or  $z = 0$  there are infinitely many. As noted in Remark 5.2, in the latter case we may replace  $V$  with  $U$ , in which case  $(z, w) = (1, 0)$  (Convention 5.3) and the maximizing pairs  $(r_U, r_V)$  are exactly those listed for Class C' in Table 3.

Combining the maximum values computed for  $\zeta = 1, j$ , and  $\zeta_{j,+}$ , we have the following: for  $\zeta \in \tilde{Z}_{1,1}$ ,

$$|f_4(\zeta)| = \max_{r_U, r_V \in S_{\mathbb{C}}^1} |\operatorname{Re}(r_V \bar{\zeta} \overline{r_U}(z + jw))| = \begin{cases} \max\{|z|, |w|\} & \text{if } \pi_\zeta = \pi_{\text{id}}, \\ \frac{1}{\sqrt{2}}(|z| + |w|) & \text{if } \pi_\zeta = \pi_{13}. \end{cases} \quad (5.40)$$

The equality  $|z|^2 + |w|^2 = 1$  implies that  $\cos^{-1}\left(\frac{|z|+|w|}{\sqrt{2}}\right) = \frac{\pi}{4} - \cos^{-1}(\max\{|z|, |w|\})$ . This fact, combined with equations (5.19), (5.40) and (5.16), yields equation (5.30).

(iv) In this case  $G_D^0 = SO(3)$ ,  $\Gamma_{J_D}^0 = \tilde{S}_3^+$ , and the set  $Z$  in Proposition 4.9 has only one element  $g$ , which we can take to be the identity. The set  $\{UR_U : U \in \widehat{G_D^0}\}$  is simply  $SO(3)$ , the inner minimum in (4.13) is 0, and  $d_{\mathcal{SR}}(X, Y) = \|\log(\Lambda D^{-1})\|$ . ■

**Remark 5.5 (Insensitivity to choice of eigen-decompositions)** By definition,  $d_{\mathcal{SR}}(X, Y)$  cannot depend on the choice of pre-images  $(U, D) \in F^{-1}(X) = \mathcal{E}_X$ ,  $(V, \Lambda) \in F^{-1}(Y) = \mathcal{E}_Y$ , that we have used to write down the formulas in Theorem 5.4. However, the assumption that  $D \in \mathcal{D}_{J_1}$  in the parts (ii) and (iii) of the theorem limits  $(U, D)$  to particular pair of connected components of  $\mathcal{E}_X$  out of the possible six. A similar comment applies in part (iii) to the choice of  $(V, \Lambda)$ . So the individual numbers  $\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}$  on the right-hand sides of (5.23) and (5.30), which represent distances between the connected component  $[(U, D)]$  and the various connected components of  $\mathcal{E}_Y$ , may depend on the choice of  $(U, D)$ , but changing  $(U, D)$  to a different pre-image of  $X$  (not necessarily with  $D \in \mathcal{D}_{J_1}$ ) must give us the same *set* of component-distances, and cannot change any of the the numbers  $\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}$  at all if the new pre-image is in the same connected component as the old. The latter *a priori* truth is reflected in the formulas given in Theorem 5.4. Although the complex numbers  $z, w$  in (5.18) depend on the choice of representatives  $(U, D) \in \mathcal{E}_X$ ,  $(V, \Lambda) \in \mathcal{E}_Y$ , when  $D$  lies in  $\mathcal{D}_{J_1}$  the quantities  $|z|, |w|$ , and  $\bar{z}w$  depend only on the connected components  $[(U, D)], [(V, \Lambda)]$ . (Changing  $(U, D)$  to  $(UR, D)$ , with  $R \in G_{\mathcal{D}_{J_1}}^0$ , changes  $(z, w)$  to  $(\xi z, \xi w)$  for some  $\xi \in S_{\mathbb{C}}^1$ ; similarly if  $\Lambda \in \mathcal{D}_{J_1}$ , then changing  $(V, \Lambda)$  to  $(VR, \Lambda)$ , with  $R \in G_{\mathcal{D}_{J_1}}^0$ , changes  $(z, w)$  to  $(\xi z, \xi w)$  for some  $\xi \in S_{\mathbb{C}}^1$ .) Thus when  $X \in \mathcal{S}_{\text{mid}}$ , and  $Y \in \mathcal{S}_{\text{mid}}$  or  $Y \in \mathcal{S}_{\text{top}}$ , in (5.18)–(5.20) we can regard  $|z|, |w|$ , and  $\bar{z}w$  as functions of a pair  $([(U, D)], [(V, \Lambda)])$  of connected components of fibers. Therefore the same is true of the quantities  $\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}$  in Theorem 5.4. (Of course, when  $Y \in \mathcal{S}_{\text{top}}$ ,  $[(V, \Lambda)] = \{(V, \Lambda)\}$ .) Furthermore, if  $D \in \mathcal{D}_{J_1}$ , then  $[(U, D)]$  and  $[(U\phi(j), D)]$  are the two connected components of  $\mathcal{E}_X$  in  $SO(3) \times \mathcal{D}_{J_1}$ . Replacing  $(U, D)$  by  $(U\phi(j), D)$  has the effect of replacing  $(z, w)$  by  $\pm(\bar{w}, -\bar{z})$ , which leaves the quantities  $\varphi, \beta, \beta'$  in (5.19)–(5.20) unchanged, and hence leaves each of the numbers  $\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}$  in (5.24)–(5.26) and (5.31)–(5.32) unchanged. The fact that replacing  $(U, D)$  by other pre-images of  $X$  cannot change the *set*  $\{\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}\}$  is also reflected, later in Theorem

6.4, by the symmetry of the last column of Table 4 under permutations of  $\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}$ .

## 6. MSSR curves for $\text{Sym}^+(3)$ in the nontrivial cases

**Notation 6.1** For  $X, Y \in \text{Sym}^+(p)$ , let  $\mathcal{M}(X, Y)$  denote the set of all MSSR curves from  $X$  to  $Y$ .

In this section, we determine the set  $\mathcal{M}(X, Y)$  for all  $X \in \mathcal{S}_{\text{mid}}, Y \in \mathcal{S}_{\text{mid}} \cup \mathcal{S}_{\text{top}}$  (what we are calling the “nontrivial cases”).

### 6.1. Explicit characterization of all MSSR curves in the nontrivial cases

For any  $X, Y \in \text{Sym}^+(p)$  and  $(U, D) \in \mathcal{E}_X$ , Proposition 4.9 assures us that every MSSR curve from  $X$  to  $Y$  corresponds to some minimal pair whose first element lies in the connected component  $[(U, D)]$ . When  $X \in \mathcal{S}_{\text{mid}}$ , by keeping track of the triples  $(\zeta, r_U, r_V)$  at which the minimum values in (5.16) are achieved, we can find all the minimal pairs in  $\mathcal{E}_X \times \mathcal{E}_Y$  whose first point lies in  $[(U, D)]$  of  $\mathcal{E}_X$ . The following corollary of Proposition 4.17 will allow us to tell when the MSSR curves corresponding to two such minimal pairs are the same.

**Corollary 6.2** *Hypotheses as in Proposition 4.17, but additionally assume that  $p = 3$ . For  $i = 1, 2$  let  $r_{U,i}, r_{V,i}$ , and  $\zeta_i$  be preimages of  $R_{U,i}, R_{V,i}$ , and  $g_i$  under  $\phi$ . Then  $\chi_1 = \chi_2$  if and only if (i)'*

$$r_{V,2} \overline{\zeta_2} \overline{r_{U,2}} = \pm r_{V,1} \overline{\zeta_1} \overline{r_{U,1}} \quad (6.1)$$

and (ii)' there exist  $\zeta \in \widehat{\Gamma}, r \in \widehat{G_{D, \Lambda_1}^0}$  such that

$$D = \pi_\zeta \cdot D, \quad (6.2)$$

$$\Lambda_2 = \pi_\zeta \cdot \Lambda_1, \quad (6.3)$$

$$\text{and } \overline{r_{U,1}} r_{U,2} = r \overline{\zeta}. \quad (6.4)$$

**Proof:** This follows immediately from Proposition 4.17 and Corollary 4.14. ■

The classification we will give of MSSR curves involves six classes of scaling-rotation curves when  $Y \in \mathcal{S}_{\text{top}}$ , and four classes when  $Y \in \mathcal{S}_{\text{mid}}$ . Not all of these classes occur for a given  $X$  and  $Y$ , and when they do occur they are not necessarily minimal. The (potentially) minimal pairs giving rise to the various classes of scaling-rotation curves can be described in terms of the data  $z, w$  and the triple  $(\zeta, r_U, r_V)$ . Our names for these classes of pairs and curves, and the data  $(\zeta, r_U, r_V)$  corresponding to each class, are listed in Table 3. For the  $\zeta$  appearing in each line of the table, the accompanying values of  $(r_U, r_V)$  are all those that minimize the arc-cosine term in the corresponding line of (5.16), provided that any unit complex number  $\hat{\xi} = \xi/|\xi|$  appearing in that line's indicated

formula for  $(r_U, r_V)$  is defined (i.e. provided  $\xi \neq 0$ ); see the proof of Theorem 6.4 in later in this section. The corresponding pairs in  $\mathcal{E}_X \times \mathcal{E}_Y$  determine a class  $\mathcal{M}_l([(U, D)], [(V, \Lambda)])$  of scaling-rotation curves, where  $l$  is the corresponding class-name appearing in Table 3. As the notation suggests, each class of curves depends only on the connected components  $[(U, D)], [(V, \Lambda)]$  in  $\mathcal{E}_X, \mathcal{E}_Y$ , although the data  $(r_U, r_V)$  for a given  $\zeta$  will depend fully on the matrices  $U, V$ . For the scaling-rotation curves in  $\mathcal{M}_l([(U, D)], [(V, \Lambda)])$  to be *minimal* there are restrictions on the component-pair  $([(U, D)], [(V, \Lambda)])$ , reflected by restrictions on  $z$  and  $w$  that depend only on these connected components; e.g. for Class B<sub>1</sub> to be minimal we need  $\operatorname{Re}(\bar{z}w) \geq 0$ , and for Class A<sub>1</sub>' to be minimal we need  $|z| \geq |w|$ . The full set of restrictions can be read off from Tables 4 and 5, which are part of Theorem 6.4 below.

In the supplementary material, we give examples, graphical illustrations, and further discussion of all ten classes of MSSR curves that arise in our classification.

**Remark 6.3** In our application of Corollary 6.2 to the proof of Theorem 6.4 below, we will have  $D \in \mathcal{D}_{J_1}$ , and hence the quaternions  $r_{U,i}, r_{V,i}$  in (6.1) and (6.4) will lie in  $S_{\mathbb{C}}^1$ . Note also that the only permutations  $\pi$  for which  $\pi \cdot D = D$  are the identity and the transposition  $\pi_{23}$ . Thus the only  $\zeta$ 's that can satisfy (6.2) are those that lie in the group  $\widehat{\Gamma}_1 = \left\{ \pm 1, \pm i, \frac{\pm 1 \pm i}{\sqrt{2}} \right\} = \{e^{2\pi i m/8} : m \in \mathbb{Z}\} \subset S_{\mathbb{C}}^1$ . However, in general the  $\zeta_i$  in (6.1) need not lie in  $\mathbb{C}$ .

**Theorem 6.4** *Assume that  $X \in \mathcal{S}_{\text{mid}}$ ,  $Y \in \mathcal{S}_{\text{top}} \cup \mathcal{S}_{\text{mid}}$ ,  $(U, D) \in \mathcal{E}_X$ ,  $(V, \Lambda) \in \mathcal{E}_Y$ , and that the first two diagonal entries of each of the matrices  $D, \Lambda$  are distinct. (Thus  $D \in \mathcal{D}_{J_1}$ , and if  $Y \in \mathcal{S}_{\text{mid}}$  then  $\Lambda \in \mathcal{D}_{J_1}$ .) Let  $l$  stand for the class-names in Table 3, and abbreviate  $\mathcal{M}_l([(U, D)], [(V, \Lambda)])$  as  $\mathcal{M}_l$ .*

(i) *Except for  $\mathcal{M}_{C'}$ , every class  $\mathcal{M}_l$ , when defined, consists of a single curve  $\chi_l = \chi_l([(U, D)], [(V, \Lambda)])$ . The class  $\mathcal{M}_{C'}$ , which we define only when  $w = 0$  or  $z = 0$ , is an infinite family of scaling-rotation curves, in natural one-to-one correspondence with a circle. The class  $\mathcal{M}_{C'}$  does not depend on the choice of components  $[(U, D)], [(V, \Lambda)] \subset SO(3) \times \mathcal{D}_{J_1}$ , so can unambiguously be written as  $\mathcal{M}_{C'}(X, Y)$ .*

(ii) *For any data-triple  $(\zeta, r_U, r_V)$  as in Table 3, let  $R_U = \phi(r_U), R_V = \phi(r_V)$ . For both  $Y \in \mathcal{S}_{\text{top}}$  and  $Y \in \mathcal{S}_{\text{mid}}$ , the pair*

$$((UR_U, D), (VR_V\phi(\zeta)^{-1}, \Lambda_{\pi_\zeta})) \in \mathcal{E}_X \times \mathcal{E}_Y \quad (6.5)$$

*is a minimal pair in each case listed in Tables 4 and 5, with  $(UR_U, D)$  lying in the connected component  $[(U, D)]$  of  $\mathcal{E}_X$ . Conversely, every minimal pair in  $\mathcal{E}_X \times \mathcal{E}_Y$  whose first point lies in  $[(U, D)]$  is given by the data in Table 3 and either Table 4 or Table 5.*

(iii) *For  $Y \in \mathcal{S}_{\text{top}}$ , depending on the value of  $Y$  the set  $\mathcal{M}(X, Y)$  can consist of one, two, three, or four curves, as detailed in Table 4. In Tables 4 and 5, note*

	Class	$\{(\zeta, r_U, r_V)\}$	$ \operatorname{Re}(r_V \bar{\zeta} \overline{r_U}(z + wj)) $
For $Y \in \mathcal{S}_{\text{top}}$ :	A <sub>1</sub>	$\{(1, \pm \hat{z}, 1)\}$	$ z $
	A <sub>2</sub>	$\{(j, \pm \hat{w}, 1)\}$	$ w $
	B <sub>1</sub>	$\{(\zeta_{j,+}, \pm \widehat{(z+w)}, 1)\}$	$\frac{1}{\sqrt{2}} z+w $
	B <sub>2</sub>	$\{(\zeta_{j,-}, \pm \widehat{(z-w)}, 1)\}$	$\frac{1}{\sqrt{2}} z-w $
	C <sub>1</sub>	$\{(\zeta_{k,+}, \pm \widehat{(z-iw)}, 1)\}$	$\frac{1}{\sqrt{2}} z-iw $
	C <sub>2</sub>	$\{(\zeta_{k,-}, \pm \widehat{(z+iw)}, 1)\}$	$\frac{1}{\sqrt{2}} z+iw $
For $Y \in \mathcal{S}_{\text{mid}}$ :	A' <sub>1</sub>	$\{(1, r, \pm r\bar{z}) : r \in S_{\mathbf{C}}^1\}$	$ z $
	A' <sub>2</sub>	$\{(j, r, \pm r\hat{w}) : r \in S_{\mathbf{C}}^1\}$	$ w $
	B'	$\{(\zeta_{j,+}, \pm (\hat{w}\hat{z})^{1/2}, \pm (\hat{w}\bar{\hat{z}})^{1/2})\}$ (all sign-combinations allowed)	$\frac{1}{\sqrt{2}}( z  +  w )$
	C'	$\{(\zeta_{j,+}, r, \pm r) : r \in S_{\mathbf{C}}^1\}$ if $(z, w) = (1, 0)$ ; class defined if $w = 0$ or $z = 0$ but left undefined otherwise.	$\frac{1}{\sqrt{2}}$

TABLE 3

Names and data for classes of pairs in  $\mathcal{E}_X \times \mathcal{E}_Y$  that, for some  $X$  in  $\mathcal{S}_{\text{mid}}$  and some  $Y$  in  $\mathcal{S}_{\text{top}}$  or  $\mathcal{S}_{\text{mid}}$ , determine at least one MSSR curve from  $X$  to  $Y$ . For any nonzero  $\xi \in \mathbf{C}$ ,  $\hat{\xi}$  is the unit complex number  $\xi/|\xi|$ , and  $\xi^{1/2}$  is an arbitrary choice of one of the two square roots of  $\xi$ . Wherever a number of the form  $\hat{\xi}$  appears in this table, the corresponding class is defined only for  $\xi \neq 0$ . In case C' we have used Convention 5.3 to simplify this line of the table; for general definition of Class C' see the proof of Theorem 5.4 in Section 5.2.3. The last column of the table is included for the proof of Theorem 5.4.

that “ $|\mathcal{M}(X, Y)| = 1$ ” means precisely that there is a unique MSSR curve from  $X$  to  $Y$ .

(iv) For  $Y \in \mathcal{S}_{\text{mid}}$ , depending on the value of  $Y$  the set  $\mathcal{M}(X, Y)$  can consist of one, two, three, or infinitely many curves, as detailed in Table 5. When  $|z| \geq |w|$  (respectively,  $|z| \leq |w|$ ), all minimal pairs in Class A'<sub>1</sub> (resp. A'<sub>2</sub>) determine the same MSSR curve, so to write down this curve it suffices to take  $r = 1$  in the data-triple for this class in Table 3.

**Remark 6.5 (Symmetries in Theorem 5.4 and Tables 4 and 5)** As noted in Remark 5.5, when  $(U, D)$  is a pre-image (eigen-decomposition) of  $X$  with  $D \in \mathcal{D}_{J_1}$ , replacing  $(U, D)$  by the pre-image  $(U\phi(j), D)$  in the other connected component of  $\mathcal{E}_X$  in  $SO(3) \times \mathcal{D}_{J_1}$  has the effect of replacing  $(z, w)$  by  $(z_{\text{new}}, w_{\text{new}}) = \pm(\bar{w}, -\bar{z})$ . Observe that  $\overline{z_{\text{new}}} w_{\text{new}} = -\bar{z}w$ , and that if  $|z| < |w|$  then  $|z_{\text{new}}| > |w_{\text{new}}|$ . Thus when  $X \in \mathcal{S}_{\text{mid}}$  we can always choose our pair of pre-images  $(U, D), (V, \Lambda)$  (with  $D \in \mathcal{D}_{J_1}$ ) to satisfy  $|z| \geq |w|$ , or  $\operatorname{Re}(\bar{z}w) \geq 0$ , or  $\operatorname{Im}(\bar{z}w) \geq 0$  (though not necessarily more than one of these inequalities at the same time). This explains the “symmetry” in Tables 4 and 5 under interchange of  $|z|$  and  $|w|$  and under sign-changes of  $\operatorname{Re}(\bar{z}w)$  and  $\operatorname{Im}(\bar{z}w)$ : we have  $\chi_{A_1}([(U\phi(j), D)], [(V, \Lambda)]) = \chi_{A_2}([(U, D)], [(V, \Lambda)])$ , and a similar relation for the class-pairs  $(B_1, B_2)$ ,  $(C_1, C_2)$ , and  $(A'_1, A'_2)$ .

**Remark 6.6 (Condition for curves in family  $\mathcal{M}_{C'}$  to be minimal)** The con-

Case	Subcase	$\mathcal{M}(X, Y)$	$ \mathcal{M}(X, Y) $
$\ell_{\text{id}} < \min\{\ell_{(13)}, \ell_{(12)}\}$	$ z  \neq  w $	$\{\chi_{A_1}\}$ if $ z  >  w $ ; $\{\chi_{A_2}\}$ if $ z  <  w $	1
	$ z  =  w $	$\{\chi_{A_1}, \chi_{A_2}\}$	2
$\ell_{(13)} < \min\{\ell_{\text{id}}, \ell_{(12)}\}$	$\text{Re}(\bar{z}w) \neq 0$	$\{\chi_{B_1}\}$ if $\text{Re}(\bar{z}w) > 0$ ; $\{\chi_{B_2}\}$ if $\text{Re}(\bar{z}w) < 0$	1
	$\text{Re}(\bar{z}w) = 0$	$\{\chi_{B_1}, \chi_{B_2}\}$	2
$\ell_{(12)} < \min\{\ell_{\text{id}}, \ell_{(13)}\}$	$\text{Im}(\bar{z}w) \neq 0$	$\{\chi_{C_1}\}$ if $\text{Im}(\bar{z}w) > 0$ ; $\{\chi_{C_2}\}$ if $\text{Im}(\bar{z}w) < 0$	1
	$\text{Im}(\bar{z}w) = 0$	$\{\chi_{C_1}, \chi_{C_2}\}$	2
$\ell_{\text{id}} = \ell_{(13)} < \ell_{(12)}$		$\{\chi_{A_m}, \chi_{B_n}\}$	
	$ z  -  w  \neq 0 \neq \text{Re}(\bar{z}w)$	$m = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ )	2
	$ z  -  w  = 0 \neq \text{Re}(\bar{z}w)$	$\{\chi_{A_1}, \chi_{A_2}, \chi_{B_n}\}$ $n = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ )	3
	$ z  -  w  \neq 0 = \text{Re}(\bar{z}w)$	$\{\chi_{A_m}, \chi_{B_1}, \chi_{B_2}\}$ $m = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ )	3
		$\{\chi_{A_m}, \chi_{C_n}\}$	
	$ z  -  w  \neq 0 \neq \text{Im}(\bar{z}w)$	$m = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	2
$\ell_{\text{id}} = \ell_{(12)} < \ell_{(13)}$		$\{\chi_{A_1}, \chi_{A_2}, \chi_{C_n}\}$	
	$ z  -  w  = 0 \neq \text{Im}(\bar{z}w)$	$n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	3
	$ z  -  w  \neq 0 = \text{Im}(\bar{z}w)$	$\{\chi_{A_m}, \chi_{C_1}, \chi_{C_2}\}$ $m = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ )	3
		$\{\chi_{B_m}, \chi_{C_n}\}$	
	$\text{Re}(\bar{z}w) \neq 0 \neq \text{Im}(\bar{z}w)$	$m = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	2
	$\text{Re}(\bar{z}w) = 0 \neq \text{Im}(\bar{z}w)$	$\{\chi_{B_1}, \chi_{B_2}, \chi_{C_n}\}$ $n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	3
$\ell_{(13)} = \ell_{(12)} < \ell_{\text{id}}$		$\{\chi_{B_n}, \chi_{C_1}, \chi_{C_2}\}$	
	$\text{Re}(\bar{z}w) \neq 0 = \text{Im}(\bar{z}w)$	$n = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ )	3
		$\{\chi_{A_1}, \chi_{B_m}, \chi_{C_n}\}$	
	$ z  \neq  w $ and $\text{Re}(\bar{z}w) \neq 0 \neq \text{Im}(\bar{z}w)$	$l = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ ), $m = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	3
	$ z  =  w $ and $\text{Re}(\bar{z}w) \neq 0 \neq \text{Im}(\bar{z}w)$	$\{\chi_{A_1}, \chi_{A_2}, \chi_{B_m}, \chi_{B_n}\}$ , $m = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	4
	$ z  \neq  w $ and $\text{Re}(\bar{z}w) = 0 \neq \text{Im}(\bar{z}w)$	$\{\chi_{A_m}, \chi_{B_1}, \chi_{B_2}, \chi_{C_n}\}$ $m = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Im}(\bar{z}w) > 0$ (resp. $< 0$ )	4
$\ell_{\text{id}} = \ell_{(13)} = \ell_{(12)}$		$\{\chi_{A_m}, \chi_{B_n}, \chi_{C_1}, \chi_{C_2}\}$	
	$ z  \neq  w $ and $\text{Re}(\bar{z}w) \neq 0 = \text{Im}(\bar{z}w)$	$m = 1$ (resp. 2) if $ z  -  w  > 0$ (resp. $< 0$ ), $n = 1$ (resp. 2) if $\text{Re}(\bar{z}w) > 0$ (resp. $< 0$ )	4

TABLE 4

The set  $\mathcal{M}(X, Y)$  of minimal smooth scaling-rotation curves from  $X$  to  $Y$  when  $X$  has exactly two distinct eigenvalues and  $Y$  has three. Data-combinations that are mutually exclusive are not shown (e.g. if  $\ell_{\text{id}} = \ell_{(13)} < \ell_{(12)}$ , it is impossible to have  $|z| - |w| = 0 = \text{Re}(\bar{z}w)$ ). In the subcase of  $\ell_{\text{id}} = \ell_{(13)} = \ell_{(12)}$  in which  $|z| = |w|$ , the hypothesis  $\text{Re}(\bar{z}w) \neq 0 \neq \text{Im}(\bar{z}w)$  is redundant; it is already implied by the case/subcase hypotheses. (This follows from Theorem 5.4; see the proof of Theorem 6.4.)



Case	Subcase	$\mathcal{M}(X, Y)$	$ \mathcal{M}(X, Y) $
$\ell_{\text{id}} < \ell_{(12)}$	$ z  \neq  w $	$\{\chi_{A'_1}\}$ if $ z  >  w $ ; $\{\chi_{A'_2}\}$ if $ z  <  w $	1
	$ z  =  w $	$\{\chi_{A'_1}, \chi_{A'_2}\}$	2
$\ell_{\text{id}} > \ell_{(12)}$	$z \neq 0 \neq w$	$\{\chi_{B'}\}$	1
	$w = 0$ or $z = 0$	$\mathcal{M}_{C'}$	$\infty$
$\ell_{\text{id}} = \ell_{(12)}$	$0 \neq  z  \neq  w  \neq 0$	$\{\chi_{A'_1}, \chi_{B'}\}$ if $ z  >  w $ ; $\{\chi_{A'_2}, \chi_{B'}\}$ if $ z  <  w $	2
	$ z  =  w $	$\{\chi_{A'_1}, \chi_{A'_2}, \chi_{B'}\}$	3
	$w = 0$ or $z = 0$	$\{\chi_{A'_1}\} \cup \mathcal{M}_{C'}$ if $w = 0$ ; $\{\chi_{A'_2}\} \cup \mathcal{M}_{C'}$ if $z = 0$	$\infty$

TABLE 5

The set  $\mathcal{M}(X, Y)$  of minimal smooth scaling-rotation curves from  $X$  to  $Y$  when each of  $X$  and  $Y$  has exactly two distinct eigenvalues. See text for notation.

ditions under which the infinite family  $\mathcal{M}_{C'}$  arises in Table 5—namely,  $\ell_{\text{id}} \geq \ell_{(12)}$  and either  $w = 0$  or  $z = 0$ —can be described more explicitly and geometrically in terms of the ellipsoids of revolution corresponding to  $X$  and  $Y$ . Recall from Remark 5.2 that “ $w = 0$  or  $z = 0$ ” is equivalent to the condition that these ellipsoids have the same axis of symmetry, and to the condition  $\varphi = 0$ . But (5.33) shows that when  $\varphi = 0$ , the condition  $\ell_{\text{id}} \geq \ell_{(12)}$  is equivalent to

$$-\log\left(\frac{d_1}{d_2}\right) \log\left(\frac{\lambda_1}{\lambda_2}\right) \geq k \frac{\pi^2}{8}. \quad (6.6)$$

In particular,  $\log\left(\frac{d_1}{d_2}\right)$  and  $\log\left(\frac{\lambda_1}{\lambda_2}\right)$  must have opposite signs for (6.6) to hold, so one of the ellipsoids must be prolate and the other oblate. Conversely, given two ellipsoids of revolution with the same axis of symmetry, one prolate and the other oblate, if their “prolateness-oblateness product” is sufficiently large—i.e. if (6.6) holds—then the set of MSSR curves from  $X$  to  $Y$  will include the 1-parameter family  $\mathcal{M}_{C'}$ . The proof below of Theorem 6.4(i) shows that for such  $X$  and  $Y$ , a choice of orientation of the common axis of symmetry naturally determines a continuous one-to-one correspondence between the “equator” of  $X$  (or  $Y$ ) and the family  $\mathcal{M}_{C'}$ . For a graphical example illustrating several members of the family  $\mathcal{M}_{C'}$  as evolutions of the  $X$ -ellipsoid to the  $Y$ -ellipsoid, see Figure 31 in the online supplement.

**Proof of Theorem 6.4.** (i) By definition, each curve-class  $\mathcal{M}_l$  is a set of (not necessarily minimal) smooth scaling-rotation curves corresponding to pairs  $((U\phi(r_U), D), (V\phi(r_V)\phi(\zeta)^{-1}, \pi_\zeta \cdot \Lambda)) \in \mathcal{E}_X \times \mathcal{E}_Y$  (where we set  $r_V = 1$  if  $Y \in \mathcal{S}_{\text{top}}$ ) for which  $r_U$  maximizes the function  $|f_1(\zeta, \cdot)|$  given by (5.34) if  $Y \in \mathcal{S}_{\text{top}}$ , or for which  $(r_U, r_V)$  maximizes the function  $|f_3(\zeta, \cdot)|$  given by (5.36) if  $Y \in \mathcal{S}_{\text{mid}}$ . In the proof of Theorem 5.4 we established that Table 3 lists all the corresponding triples  $(\zeta, r_U, r_V)$ , with the exception that for class  $C'$  we followed Convention 5.3 and listed the corresponding triples only for the case  $(z, w) = (1, 0)$  (see Remark 5.2). For  $i \in \{1, 2\}$  let  $(\zeta, r_{U,i}, r_{V,i})$  be two such

triples listed in Table 3 corresponding to the same class  $\mathcal{M}_l$ , and let  $\chi_i$  be the MSSR curves they determine.

First assume that  $l \neq C'$ . Then  $r_{U_2} = \pm r_{U_1}$  and  $r_{V_1} = \pm r_{V_2}$ , so  $\phi(r_{U_2}) = \phi(r_{U_1})$  and  $\phi(r_{V_1}) = \phi(r_{V_2})$ . Hence the minimal pair in  $(SO \times \text{Diag}^+)(3)$  determined by  $(\zeta, r_{U,i}, r_{V,i})$  is the same for both values of  $i$ , so  $\chi_2 = \chi_1$ . Thus  $\mathcal{M}_l$  consists of a single curve.

Now assume that the  $(\zeta, r_{U,i}, r_{V,i})$  are associated with class  $C'$  and that  $(z, w) = (1, 0)$ . Then  $(\zeta, r_{U,i}, r_{V,i}) = (\zeta_{j,+}, r_i, \epsilon_i r_i)$  for some  $r_i \in S_{\mathbf{C}}^1$  and  $\epsilon_i \in \{\pm 1\}$ . A straightforward computation yields  $r_{V,i} \overline{\zeta_{j,+}} \overline{r_{V,i}} = \epsilon_i \frac{1}{\sqrt{2}} (1 - (r_i)^2 j)$ . Thus by Corollary 6.2, a necessary condition to have  $\chi_2 = \chi_1$  is

$$1 - (r_2)^2 j = \pm(1 - r_1^2 j), \quad (6.7)$$

But  $(r_i)^2 j \in \text{span}\{j, k\}$ , which holds only if  $r_2 = \pm r_1$ . Thus if  $r_2 \neq \pm r_1$ , then  $\chi_2 \neq \chi_1$ . Conversely, suppose that  $r_2 = \epsilon r_1$ , where  $\epsilon = \pm 1$ . Then (6.7) holds,  $\overline{r_{U,1}} r_{U,2} = \epsilon$ , and (6.2)–(6.4) are satisfied with  $\zeta = 1$  and  $r = \epsilon$ . Corollary 6.2 then implies that  $\chi_2 = \chi_1$ .

Thus for triples  $(\zeta_{j,+}, r_{U,i}, r_{V,i})$  associated with class  $C'$ , a necessary and sufficient condition for  $\chi_1, \chi_2$  to coincide (following Convention 5.3) is  $r_{U,2} = \pm r_{U,1}$ , which is equivalent to  $R_{U,1} = R_{U,2}$  in  $SO(3)$ . Since  $R_{U,i} \in G_D^0$ , the preceding sets up a one-to-one correspondence between  $\mathcal{M}_{C'}$  and the circle  $G_D^0$ :

$$\left. \begin{array}{ll} (R \in G_D^0) & \longleftrightarrow F_1(R) := \chi_{C'}^R \\ \text{where } \chi_{C'}^R & = \text{the SR curve } [0, 1] \rightarrow \text{Sym}^+(3) \text{ determined by} \\ & \text{the minimal pair } ((UR, D), (UR\phi(\zeta_{j,+})^{-1}, \pi_{13} \cdot \Lambda)). \end{array} \right\} \quad (6.8)$$

Note the the map  $G_D^0 \times [0, 1] \rightarrow \text{Sym}^+(3)$ ,  $(R, t) \mapsto \chi_{C'}^R(t)$ , is continuous, hence uniformly continuous since  $G_D^0 \times [0, 1]$  is compact. Thus the injective map  $F_1 : G_D^0 \rightarrow C([0, 1], \text{Sym}^+(3))$  (the space of continuous maps  $[0, 1] \rightarrow \text{Sym}^+(3)$ ) is continuous, hence a homeomorphism onto its image (since  $G_D^0$  is compact and  $C([0, 1], \text{Sym}^+(3))$  is Hausdorff), which is  $\mathcal{M}_{C'}$ . Therefore, in this natural topology,  $\mathcal{M}_{C'}$  is homeomorphic to a circle.

While the above map  $F_1$  explicitly parametrizes  $\mathcal{M}_{C'}$  by the circle  $G_D^0$ , this parametrization is not canonical—it depends on several non-unique choices, such as a particular matrix  $U \in SO(p)$  among all those that satisfy  $UDU^T = X$ , and our choice of representative  $\zeta_{j,+}$  of the double-coset  $(\widehat{\Gamma_D^0}, \widehat{\Gamma_\Lambda^0})$  double-coset (in  $\widehat{\Gamma}$ ) in which  $\zeta_{j,+}$  lies. There is a more directly geometric parametrization of  $\mathcal{M}_{C'} = \mathcal{M}_{C'}(X, Y)$ , which we exhibit next, by a circle in  $\mathbf{R}^3$  determined by the ellipsoids  $\Sigma_X, \Sigma_Y$  to which  $X, Y$  correspond.

Recall that under the Class  $C'$  hypotheses ( $w = 0$  or  $z = 0$ ),  $X$  and  $Y$  have the same, unique, axis of circular symmetry  $L$  (see Remark 6.6), and hence also have a common “equatorial plane”  $L^\perp$ . For  $t \in [0, 1]$  and  $R \in G_D^0$ , let  $\Sigma_t^R$  be the ellipsoid in  $\mathbf{R}^3$  corresponding to  $\chi_{C'}^R(t)$ ; note that  $\Sigma_0^R = \Sigma_X$  and  $\Sigma_1^R = \Sigma_Y$  for all  $R$ .

Let  $Q = \log(\phi(\zeta_{j,+}))' = \log(\phi(\zeta_{j,-}))$ ; explicitly,

$$Q = \frac{\pi}{2} \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

(the matrix  $\phi(\zeta_{j,-})$  is given in Table 2). For  $R \in G_D^0$  let  $A(R) = URQ(UR)^{-1}$ . Then  $A = \log(UR\phi(\zeta_{j,+})^{-1}(UR)^{-1})$ , and from equation(s) (4.5)–(4.6) we have

$$\begin{aligned} \chi_{C'}^R(t) &= e^{tA(R)}URD^{1-t}(\pi_{13}\cdot\Lambda)^t(e^{tA(R)}UR)' \\ &= U_R(t)D^{1-t}(\pi_{13}\cdot\Lambda)^tU_R(t)' \end{aligned} \quad (6.9)$$

where  $U_R(t) = e^{tA(R)}UR = URe^{tQ}$ . Let  $\mathbf{e}_1 = (1, 0, 0)'$ , let  $\epsilon \in \{\pm 1\}$ , and define  $\gamma_R(t) = U_R(t)\epsilon\mathbf{e}_1$ . For all  $R \in G_D^0$ , the vector  $v_0 = \gamma_R(0)$  is one of the two unit vectors lying on the axis  $L$ , and  $\gamma_R(t)$  is a unit vector lying on one of the principal axes of  $\Sigma_t^R$ ; equivalently, a unit eigenvector of  $\chi_{C'}^R(t)$ . For each  $R$ , the inner product of  $v_0$  with  $\gamma_R(1)$  is

$$(UR\mathbf{e}_1) \cdot (UR\phi(\zeta_{j,-})\mathbf{e}_1) = \mathbf{e}_1 \cdot (\phi(\zeta_{j,-})\mathbf{e}_1) = (1, 0, 0) \cdot (0, 0, 1) = 0.$$

Hence  $\gamma_R(1)$  lies in the unit circle  $C$  in the equatorial plane  $L^\perp$ . It is easily checked that the continuous map  $F_2 := F_{2,v_0} : G_D^0 \rightarrow C$  given by  $F_2(R) = \gamma_R(1)$  is a bijection, hence a homeomorphism. Thus the map  $F_{v_0} := F_1 \circ (F_{2,v_0})^{-1} : C \rightarrow \mathcal{M}_{C'}$  parametrizes  $\mathcal{M}_{C'}(X, Y)$  by the circle  $C$ .

One can easily check that there is at most one  $t \in (0, 1)$  for which the eigenvalues of  $\chi_{C'}^R(t)$  are not all distinct. Thus  $\gamma_R$  is the unique continuous map  $[0, 1] \rightarrow \mathbf{R}^3$  such that  $\gamma_R(0) = v_0$ ,  $\gamma_R(1) = F_2(R)$ , and  $\gamma_R(t)$  is a unit eigenvector of  $\chi_{C'}^R(t)$  for all  $t \in [0, 1]$ . Hence for each  $\chi \in \mathcal{M}_{C'}(X, Y)$ , there is a unique continuous map  $\tilde{\gamma}_\chi = \tilde{\gamma}_{\chi, v_0} : [0, 1] \rightarrow \mathbf{R}^3$  such that  $\tilde{\gamma}_\chi(0) = v_0$  and  $\tilde{\gamma}_\chi(t)$  is a unit eigenvector of  $\chi(t)$  for all  $t \in [0, 1]$ .

This characterization shows that the parametrization  $F_{v_0} : C \rightarrow \mathcal{M}_{C'}(X, Y)$  is canonical up to the choice  $v_0$  of one of the two unit vectors  $L$ . Given  $v_0$  and a vector  $w \in C$ , there is a unique  $\chi = \chi_{w, v_0} \in \mathcal{M}_{C'}(X, Y)$  such that the curve  $\tilde{\gamma}_\chi$  defined above has  $\tilde{\gamma}_\chi(0) = v_0$  and  $\tilde{\gamma}_\chi(1) = w$ . Moreover,  $\tilde{\gamma}_{\chi, -v_0}(1) = -\tilde{\gamma}_{\chi, v_0}(1)$ , so the two parametrizations are simply related to each other  $(F_{-v_0})^{-1} = -(F_{v_0})^{-1}$ .

(ii) Our proof of Theorem 5.4 established that all the MSSR curves from  $X$  to  $Y$  are accounted for by the curves coming from minimal pairs in the classes listed in Table 3. The first element  $(UR_U, D)$  of each such pair lies in  $[(U, D)]$ , since  $R_U \in G_D^0$ .

It remains only to establish that all MSSR curves are accounted for by one of the (sub)cases listed in Table 4 or Table 5, and that necessary and sufficient conditions for the curve(s) in a given class  $\mathcal{M}_l$  to be minimal are the conditions that can be read off from Table 4 if  $Y \in \mathcal{S}_{\text{top}}$ , or Table 5 if  $Y \in \mathcal{S}_{\text{mid}}$ . (For example, if  $Y \in \mathcal{S}_{\text{top}}$ , to read off from Table 4 the conditions for the (unique) curve  $\chi_{A_1}$  in  $\mathcal{M}_{A_1}$  to be minimal, we simply take the union of all the cases for which  $\chi_{A_1}$  is an element of  $\mathcal{M}(X, Y)$ , as indicated by the third column of the table. These conditions reduce to:  $|z| \geq |w|$  and  $\ell_{\text{id}} \leq \min\{\ell_{(13)}, \ell_{(12)}\}$ .)

First assume that  $Y \in \mathcal{S}_{\text{top}}$ . Equations (5.27)–(5.29) show that no nonvacuous subcases have been omitted in Table 4. (For example, if  $|z| - |w| = 0 = \text{Re}(\bar{z}w)$  then  $\varphi = \frac{\pi}{4} = \beta$ , so (5.27) shows that  $\ell_{\text{id}}^2 - \ell_{(13)}^2 \neq 0$ , since, by hypothesis,  $d_1 \neq d_2$  and  $\lambda_1 \neq \lambda_3$ ; thus for the two cases in Table 4 in which  $\ell_{\text{id}} = \ell_{(13)}$ , there are no “ $|z| - |w| = 0 = \text{Re}(\bar{z}w)$ ” subcases. In the last case in the table, equations (5.27)–(5.29) show that no two of the three angles  $\varphi, \beta, \beta'$  can be equal, and hence that if  $|z| = |w|$  [equivalently,  $\varphi = \frac{\pi}{4}$ ], then automatically  $\text{Re}(\bar{z}w) \neq 0 \neq \text{Im}(\bar{z}w)$ ; else we would have  $\beta = \frac{\pi}{4}$  or  $\beta' = \frac{\pi}{4}$ . Thus the hypothesis  $\text{Re}(\bar{z}w) \neq 0 \neq \text{Im}(\bar{z}w)$  in the  $|z| = |w|$  subcase of  $\ell_{\text{id}} = \ell_{(13)} = \ell_{(12)}$  in which  $|z| = |w|$  is redundant, as asserted in the table’s caption.) Hence every MSSR curve from  $X$  to  $Y$  occurs in one of the subcases listed in column 2 of Table 4.

For  $l \in \{A_1, A_2, B_1, B_2, C_1, C_2\}$ , let  $\zeta_l$  be the element of  $\tilde{Z}_{1,*}$  that appears in the triples to the right of class-name  $l$  in Table 3, and define  $\ell_l \geq 0$  by

$$\ell_l^2 = 4k \left( \cos^{-1} |f_2(\zeta_l)| \right)^2 + \|\log(\Lambda_{\pi_{\zeta_l}} D^{-1})\|^2, \quad (6.10)$$

where  $f_2$  is as in the proof of Theorem 5.4; cf. (5.16). Then  $\ell_{\text{id}} = \min\{\ell_{A_1}, \ell_{A_2}\}$ ,  $\ell_{(13)} = \min\{\ell_{B_1}, \ell_{B_2}\}$ , and  $\ell_{(12)} = \min\{\ell_{C_1}, \ell_{C_2}\}$ . A set of necessary and sufficient conditions to have  $d_{\mathcal{SR}}(X, Y) = \ell_{A_i}$  (respectively  $\ell_{B_i}, \ell_{C_i}$ ) is: (a)  $\ell_{A_i} \leq \ell_{A_{i'}}$  (resp.  $\ell_{B_i} \leq \ell_{B_{i'}}$ ,  $\ell_{C_i} \leq \ell_{C_{i'}}$ ), where  $\{i, i'\} = \{1, 2\}$ , and (b)  $\min\{\ell_{\text{id}}, \ell_{(13)}, \ell_{(12)}\} = \ell_{\text{id}}$  (resp.  $\ell_{(13)}, \ell_{(12)}$ ).

For  $l = A_1$  and  $l = A_2$  the contributions to  $\ell_l$  from the term involving  $D$  on the right-hand side of (6.10) are identical, so  $\ell_{A_1} \leq \ell_{A_2}$  if and only if  $|f_2(1)| \geq |f_2(j)|$ . Thus,  $\ell_{A_1} \leq \ell_{A_2} \iff |z| \geq |w|$ . Similarly,  $\ell_{B_1} \leq \ell_{B_2} \iff |z + w| \geq |z - w| \iff \text{Re}(\bar{z}w) \geq 0$ , and  $\ell_{C_1} \leq \ell_{C_2} \iff |z - iw| \geq |z + iw| \iff \text{Im}(\bar{z}w) \geq 0$ . Note that  $\max\{|z|, |w|\}$ ,  $\max\{|z + w|, |z - w|\}$ , and  $\max\{|z + iw|, |z - iw|\}$  are all strictly positive. Hence, if  $d_{\mathcal{SR}}(X, Y) = \ell_l$ , then  $f_2(\zeta_l) \neq 0$ ,  $f_2(\zeta_l)$  is defined, and the curve  $\chi_l$  associated with the data listed in Table 3 is defined.

Thus, for  $Y \in \mathcal{S}_{\text{top}}$ , all MSSR curves from  $X$  to  $Y$  are accounted for in Table 4, and in each case listed in the table, a curve  $\chi_l$  is minimal (where  $l \in \{A_1, A_2, B_1, B_2, C_1, C_2\}$ ) if and only if the conditions indicated in the table are satisfied.

Now assume that  $Y \in \mathcal{S}_{\text{mid}}$ . Analogously to the case  $Y \in \mathcal{S}_{\text{top}}$ , define  $\ell_l \geq 0$  by

$$\ell_l^2 = 4k \left( \cos^{-1} |f_4(\zeta_l)| \right)^2 + \|\log(\Lambda_{\pi_{\zeta_l}} D^{-1})\|^2, \quad (6.11)$$

where  $l \in \{A_1, A_2, B_1, B_2, C_1, C_2\}$ ,  $\zeta_l$  is the element of  $\tilde{Z}_{1,*}$  that appears in the triples to the right of class-name  $l$  in Table 3, and  $f_4$  is as in the proof of Theorem 5.4 (again cf. (5.16)). Then  $\ell_{\text{id}} = \min\{\ell_{A'_1}, \ell_{A'_2}\}$ . A set of necessary and sufficient conditions to have  $d_{\mathcal{SR}}(X, Y) = \ell_{A'_i}$  is: (a)'  $\ell_{A'_i} \leq \ell_{A'_{i'}}$ , where  $\{i, i'\} = \{1, 2\}$ , and (b)'  $\ell_{\text{id}} \leq \ell_{(13)}$ . Noting that exactly one of the classes  $B'$  and  $C'$  is defined for a given  $Y$ , a necessary and sufficient conditions to have  $d_{\mathcal{SR}}(X, Y) = \ell_{B'}$  (respectively  $\ell_{C'}$ ) is  $\ell_{(13)} \leq \ell_{\text{id}}$ .

The same reasoning used in the case  $Y \in \mathcal{S}_{\text{top}}$  shows now that  $\ell_{A'_1} \leq \ell_{A'_2}$  if and only if  $|z| \geq |w|$ , and that if  $d_{\mathcal{SR}}(X, Y) = \ell_l$ , then the curve-class  $\mathcal{M}_l$

associated with the data listed in Table 3 is defined. It follows that for  $Y \in \mathcal{S}_{\text{mid}}$ , all MSSR curves from  $X$  to  $Y$  are accounted for in Table 5, and in each case listed in the table, the curve(s)  $\chi$  in the class  $\mathcal{M}_l$  (where  $l \in \{A'_1, A'_2, B', C'\}$ ) is/are minimal if and only if the conditions indicated in the table are satisfied (modulo Convention 5.3 in the case of class  $C'$ ).

(iii) Since we have now established that  $\mathcal{M}(X, Y)$  consists of precisely those curves listed in Table 4 for the subcase corresponding to the given data  $((U, D), (V, \Lambda))$ , it suffices to show that if  $\chi_1, \chi_2$  are MSSR curves in distinct classes  $l_1, l_2 \in \{A_1, A_2, B_1, B_2, C_1, C_2\}$ , then  $\chi_1 \neq \chi_2$ .

Given such  $l_1, l_2$ , for  $i \in \{1, 2\}$  let  $(\zeta_i, r_{U,i}, r_{V,i})$  be a triple from Table 3 correspond to class  $l_i$ . Since  $r_{V,1} = 1 = r_{V,2}$  for all such triples in all classes corresponding to  $Y \in \mathcal{S}_{\text{top}}$ , we may rewrite (6.1) as  $\overline{\zeta_1} \zeta_2 = \pm \overline{r_{U,1}} r_{U,2}$ . But  $\overline{r_{U,1}} r_{U,2} \in \mathbf{C}$ , so by Corollary 6.2 a necessary condition to have  $\chi_1 = \chi_2$  is

$$\overline{\zeta_1} \zeta_2 \in \mathbf{C}. \quad (6.12)$$

We compute the following:

$$\begin{aligned} (\zeta_1, \zeta_2) = (1, j) &\implies \overline{\zeta_1} \zeta_2 = j, \\ (\zeta_1, \zeta_2) = (\zeta_{j,+}, \zeta_{j,-}) &\implies \overline{\zeta_1} \zeta_2 = -j, \\ (\zeta_1, \zeta_2) = (\zeta_{k,+}, \zeta_{k,-}) &\implies \overline{\zeta_1} \zeta_2 = -k, \\ (\zeta_1, \zeta_2) \in \{1, j\} \times \{\zeta_{j,\pm}\} &\implies \overline{\zeta_1} \zeta_2 \in \left\{ \frac{\pm 1 \pm j}{\sqrt{2}} \right\}, \\ (\zeta_1, \zeta_2) \in \{1, j\} \times \{\zeta_{k,\pm}\} &\implies \overline{\zeta_1} \zeta_2 \in \left\{ \frac{1 \pm k}{\sqrt{2}}, \frac{\pm i - j}{\sqrt{2}} \right\}, \\ (\zeta_1, \zeta_2) \in \{\zeta_{j,\pm}\} \times \{\zeta_{k,\pm}\} &\implies \overline{\zeta_1} \zeta_2 \in \left\{ \frac{1 \pm i \pm j \pm k}{2} \right\}. \end{aligned} \quad (6.13)$$

Since  $\overline{\zeta_1} \zeta_2 \notin \mathbf{C}$  in every case, it follows that  $\chi_1 \neq \chi_2$ .

(iv) Analogously to part (iii), since we have now established that  $\mathcal{M}(X, Y)$  consists of precisely those curves listed in Table 5 for the subcase corresponding to the given data  $((U, D), (V, \Lambda))$ , and that  $\mathcal{M}_{C'}$  (when defined) contains infinitely many curves, it suffices to show that if  $\chi_1, \chi_2$  are MSSR curves in distinct classes  $l_1, l_2 \in \{A'_1, A'_2, B', C'\}$ , then  $\chi_1 \neq \chi_2$ . Since exactly one of the classes  $\mathcal{M}_{B'}, \mathcal{M}_{C'}$  is nonempty, we do not need to consider the case  $\{l_1, l_2\} = \{B', C'\}$ . Because of Convention 5.3 in Remark 5.2, we also do not need to consider the case  $\{l_1, l_2\} = \{A'_2, C'\}$ . Thus we need only consider the case-pairs  $(l_1, l_2) \in \{(A'_1, A'_2), (A'_1, B'), (A'_1, C'), (A'_2, B')\}$ .

Given such  $(l_1, l_2)$ , for  $i \in \{1, 2\}$  let  $(\zeta_i, r_{U,i}, r_{V,i})$  again be a data-triple from Table 3 correspond to class  $l_i$ . By Corollary 6.2, to show  $\chi_1 \neq \chi_2$  it suffices to show that (6.1) is not satisfied. If  $l_1 = A'_1$  then  $\zeta_1 = 1$ , and (6.1) cannot be satisfied unless  $\zeta_2 \in \mathbf{C}$ , which does not hold since  $l_2 \neq A'_1$ . For the case  $(l_1, l_2) = (A'_2, B')$ , if (6.1) were satisfied we would have  $\overline{\zeta_{j,+}} = \xi_1 j \xi_2$  for some  $\xi_1, \xi_2 \in \mathbf{C}$ , an impossibility since  $\xi_1 j \xi_2 = \xi_1 \overline{\xi_2} j \in \mathbf{C}j = \text{span}\{j, k\}$ . ■

In the supplementary material, Sections 2.2 and 2.3 provide further discussion and graphical examples of all the cases  $A_i, B_i, C_i, A'_i, B', C'$ .

### 6.2. Algorithm for computing MSSR curves for $p = 3$ in the nontrivial cases

Let  $X, Y \in \text{Sym}^+(3)$  be as in Theorem 6.4. Starting with eigen-decompositions  $(U, D)$  of  $X$ ,  $(V, \Lambda)$  of  $Y$ , an algorithm to compute all the MSSR curve(s) from  $X$  to  $Y$  is as follows. This algorithm applies *only* when  $p = 3$ , and only to the nontrivial cases. However, we mention that for any  $p$ , a non-identity matrix  $R \in O(p)$  is an involution if and only if  $R = R^T$ ; thus testing in Step 1 whether a given  $U^{-1}VI_\sigma$  is an involution is very simple.

- Step 1. If  $U^{-1}V$  is not an involution, proceed to Step 2. If  $U^{-1}V$  is an involution, find an even sign-change matrix  $I_\sigma$  (of which there are only three) for which  $d_{SO(3)}(U^{-1}VI_\sigma, I) < d_{SO(3)}(U^{-1}V, I)$ . Proposition 4.13(a) implies that at least one of the three non-identity even sign-change matrices will have this property. Because  $p = 3$  here, this property is equivalent to  $U^{-1}VI_\sigma$  not being an involution (see Remark 7.8). The pair  $(VI_\sigma, \Lambda)$  is still a pre-image of  $Y$  since the action of sign-change matrices on diagonal matrices is trivial. Replace  $V$  by  $VI_\sigma$ , renamed to  $V$ . Proceed to Step 2.
- Step 2. Find  $\theta \in [0, \pi)$  and a unit vector  $\tilde{a} \in \mathbf{R}^3$  such that  $U^{-1}V = R_{\theta, \tilde{a}}$ . There is a unique such  $\theta$  and, if  $\theta \neq 0$ , a unique such  $\tilde{a}$ ; writing  $R = U^T V$  these can be computed using

$$\theta = \cos^{-1} \frac{\text{tr}(R) - 1}{2}, \quad (6.14)$$

$$\tilde{a} = \begin{cases} \frac{1}{2 \sin \theta} (R_{32} - R_{23}, R_{13} - R_{31}, R_{21} - R_{12})^T & \text{if } \theta \neq 0, \\ \mathbf{0} & \text{if } \theta = 0. \end{cases} \quad (6.15)$$

(Equations (6.14)–(6.15) are consequences of the well-known “Rodrigues formula”.)

- Step 3. Define  $z, w \in \mathbf{C}$  by  $z + wj = s(U^{-1}V)$ , where  $s : SO(3)_{<\pi} \rightarrow S^3$  is the map given by (5.2). The “minimal classes”, i.e. the curve-classes containing an element of  $\mathcal{M}(X, Y)$ , as well as the cardinality of  $\mathcal{M}(X, Y)$ , can then be read off from Table (4) if  $Y \in \mathcal{S}_{\text{top}}$ , or Table (5) if  $Y \in \mathcal{S}_{\text{mid}}$ . (If  $Y \in \mathcal{S}_{\text{top}}$ , first compute the numbers  $\ell_{\text{id}}, \ell_{(13)},$  and  $\ell_{(12)}$ , defined in (5.24)–(5.26), to use Table 4.) The appropriate line of Table 3 then gives the pairs  $(r_U, r_V) \in S_{\mathbf{C}}^1 \times S_{\mathbf{C}}^1$  for each curve-class. The remaining steps of this algorithm are applied to each minimal class.

Note that for any class other than  $C'$ , all the  $(r_U, r_V)$  pairs in Table 3 determine the same scaling-rotation curve, so just choose one pair from this line of the table. If the data are in class  $C'$ , there will be one MSSR curve for each  $r \in S_{\mathbf{C}}^1$ , but the  $\pm$  sign in the table can be ignored (treated as  $+$ ), since the sign does not affect the image under  $\phi$ .

- Step 4. For the chosen  $(r_U, r_V)$  in each minimal class (there will only be one in each class except for Class C'), compute the rotations  $R_U = \phi(r_U)$ ,  $R_V = \phi(r_V)$  from the unit complex numbers  $r_U, r_V$  using the general formula

$$\phi(e^{ti}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos 2t & -\sin 2t \\ 0 & \sin 2t & \cos 2t \end{bmatrix} \quad \text{for } t \in \mathbf{R}. \quad (6.16)$$

(Note that if we identify the  $x_2x_3$  plane with  $\mathbf{C}$  via  $(x_2, x_3) \leftrightarrow x_2 + x_3i$ , then for  $\xi \in S_{\mathbf{C}}^1$  the lower right  $2 \times 2$  submatrix of  $\phi(\xi)$  corresponds simply to multiplication by  $\xi^2$ . In Case B' this conveniently “undoes” the square roots in Table 3; for example, if  $r_U = \pm(\hat{z}\hat{w})^{1/2}$ , then  $\phi(r_U)$  is the rotation about the  $x_1$  axis that corresponds to multiplying  $x_2 + x_3i$  by  $\hat{z}\hat{w}$ .)

- Step 5. Read off the value of  $\phi(\zeta)$  from Table 2. Then plug this and the values of  $(R_U, R_V)$  computed in Step 4 into (6.5), yielding (for each of these pairs) the endpoints of a geodesic from  $\mathcal{E}_X$  to  $\mathcal{E}_Y$  whose projection to  $\text{Sym}^+(3)$  is an MSSR curve.
- Step 6. For each of the endpoint-pairs computed in Step 5, writing the endpoints as  $(U_1, D) \in \mathcal{E}_X, (V_1, \Lambda_1) \in \mathcal{E}_Y$ , set  $A = \log(U_1^{-1}V_1), L = \log(D^{-1}\Lambda_1)$ . Then use formulas (4.5) and (4.6) (with  $U_1$  playing the role of  $U$  in these formulas) to compute the formula for the corresponding MSSR curve  $\chi : [0, 1] \rightarrow \text{Sym}^+(p)$ .

**Remark 6.7** For the case in which each of  $X$  and  $Y$  has exactly two distinct eigenvalues, this algorithm for computing closed-form expressions for MSSR curves in the  $p = 3$  nontrivial cases replaces the numerical algorithm in [14] described therein after Theorem 4.3.

## 7. Appendix: Sign-change reducibility and distance between subspaces of $\mathbf{R}^p$

In this Appendix we prove the results stated in Section 4.3, and present some results that may be of independent interest.

Recall from Section 4.3 that two points  $U, V \in SO(p)$  are geodesically antipodal if and only if  $V^{-1}U$  is an involution. Since  $d_{SO(p)}(U, V) = d_{SO(p)}(V^{-1}U, I)$ , the set of distances between geodesically antipodal points in  $SO(p)$  is the same as the set of distances between the identity and involutions. Thus to understand which (if any) geodesically antipodal pairs  $(U, V)$  in  $SO(p)$  are sign-change reducible, it suffices to study the case  $(U, V) = (R, I)$ , where  $R$  is an involution.

Thus we focus on involutions in Sections 7.1–7.3. Section 7.1 reviews the (un-oriented) “normal form” of an element of  $SO(p)$ , and how this is related to distance to the identity. Section 7.2 defines sign-change reducibility for elements of  $SO(p)$ , discusses the one-to-one correspondence between the set of involutions (denoted  $\text{Inv}(p)$ ) and the disjoint union of Grassmannians  $\text{Gr}_m(\mathbf{R}^p)$  ( $m$  even and positive), and states several results concerning sign-change reducibility of involutions and its relation to distances between certain subspaces of  $\mathbf{R}^p$ . Proposition 7.7 states the equivalence between a sign-change-reducibility question and

a question purely about the geometry of  $\text{Gr}_m(\mathbf{R}^p)$  (endowed with a standard metric). In Section 7.3 we establish an unexpected (to us) half-angle formula: for any two involutions  $R_1, R_2 \in SO(p)$ , each of the principal angles between the  $(-1)$ -eigenspaces of  $R_1$  and  $R_2$  is exactly half a correspondingly indexed normal-form angle of  $RI_\sigma$  (Corollary 7.13). This relationship holds whether or not the dimensions of the  $(-1)$ -eigenspaces are equal. When the dimensions *are* equal, we use this relationship to show, without using any Riemannian geometry, that the correspondence between  $\text{Gr}_m(\mathbf{R}^p)$  and a connected component  $\text{Inv}_m(p)$  is an isometry up to a constant factor of 2 (Corollary 7.14; see Remark 7.15 for an additional interpretation). We then use this fact to help prove the results stated in Section 7.2, as well as Proposition 4.13. Finally, Section 7.4 gives the proof of Proposition 4.15.

### 7.1. Normal form and distance to the identity in $SO(p)$ .

Let  $k = \lfloor \frac{p}{2} \rfloor$ . Recall that every  $R \in SO(p)$  has a *normal form*: a block-diagonal matrix that, for  $p$  even, is of the form

$$R(\theta_1, \dots, \theta_k) = \begin{bmatrix} C(\theta_1) & & & & \\ & C(\theta_2) & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & C(\theta_k) \end{bmatrix}, \quad (7.1)$$

where

$$C(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \quad (7.2)$$

and where  $\theta_i \in [0, \pi]$ ,  $1 \leq i \leq k$ . For the odd- $p$  case, the normal-form matrix is the matrix (7.1) with one more row and column appended, and with a 1 in the lower right-hand corner (and zeroes everywhere else in the last row and column). In this case we define  $\theta_{k+1} = 0$ , so that for both even and odd  $p$  we can use the notation  $R(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$  for the normal form.

Note that

$$C(\theta) = \exp(\theta J) \quad \text{where} \quad J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \quad (7.3)$$

For each  $R \in SO(p)$  there exists an orthonormal basis of  $\mathbf{R}^p$  with respect to which the linear transformation  $\mathbf{R}^p \rightarrow \mathbf{R}^p$ ,  $v \mapsto Rv$ , has matrix  $R(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$ . Thus there exists  $Q \in O(p)$  such that

$$R = QR(\theta_1, \dots, \theta_{\lceil p/2 \rceil})Q^{-1}. \quad (7.4)$$

The normal form of a given  $R$  is unique up to ordering of the blocks; the multi-set  $\{\theta_1, \dots, \theta_{\lceil p/2 \rceil}\}$  is uniquely determined by  $R$ . From (7.2) and (7.4) we have

$$R = Q \exp(A(\theta_1, \dots, \theta_{\lceil p/2 \rceil}))Q^{-1} = \exp(QA(\theta_1, \dots, \theta_{\lceil p/2 \rceil})Q^{-1}) \quad (7.5)$$



where  $A(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$  is the block-diagonal matrix obtained by replacing  $C(\theta_i)$  by  $\theta_i J$  in (7.1),  $1 \leq i \leq \lceil p/2 \rceil$ , and, in the odd- $p$  case, replacing the 1 in the lower right-hand corner by 0. Since the normal form is unique up to block-ordering, it follows that

$$d_{SO(p)}(R, I)^2 = \sum_{i=1}^{\lfloor p/2 \rfloor} \theta_i^2 = \sum_{i=1}^{\lceil p/2 \rceil} \theta_i^2 \quad (7.6)$$

Furthermore, from (7.4) and (7.2) it follows that

$$R_{\text{sym}} := \frac{R + R^T}{2} = Q \begin{bmatrix} \cos \theta_1 & I_{2 \times 2} & & & \\ & \cos \theta_2 & I_{2 \times 2} & & \\ & & \ddots & \ddots & \\ & & & \ddots & \cos \theta_k & I_{2 \times 2} \end{bmatrix} Q^{-1} \quad (7.7)$$

if  $p$  is even; for odd  $p$  we again just append one more row and column of the middle matrix, with a 1 in the lower right-hand corner. Hence the values  $\cos \theta_i$  (and therefore the values  $\theta_i \in [0, \pi]$ ) can be recovered from  $R$  as the eigenvalues of  $R_{\text{sym}}$ , with the multiplicity of an eigenvalue  $\lambda$  of  $R_{\text{sym}}$  equal to twice the multiplicity  $m_\lambda$  of  $\lambda$  in the list  $\cos \theta_1, \dots, \cos \theta_k$  in the even- $p$  case; for odd  $p$  the only difference is that multiplicity of the eigenvalue 1 of  $R_{\text{sym}}$  is  $2m_1 + 1$ .

Writing  $R \in SO(p)$  in the form (7.4), it is easily seen that  $R$  is an involution if and only if (i) for each  $i$ ,  $\theta_i$  is either 0 or  $\pi$ , and (ii)  $\theta_i = \pi$  for at least one  $i$ . For such  $R$ , if  $\theta_i = \pi$  for exactly  $j$  values of  $i$ , then  $\|A(\theta_1, \dots, \theta_{\lceil p/2 \rceil})\|^2 = j\pi^2$ . Hence

$$\{d_{SO(p)}(R, I) : R \in SO(p), R \text{ an involution}\} = \{\sqrt{j}\pi : 1 \leq j \leq \lfloor \frac{p}{2} \rfloor\}. \quad (7.8)$$

Using (7.5) it can also be shown that for every non-involution  $R \in SO(p)$ , there is a unique  $A \in \mathfrak{so}(p)$  of smallest norm such that  $\exp(A) = R$ .

### Notation 7.1

1. Given  $R \in SO(p)$  and angles  $\theta_1, \dots, \theta_{\lceil p/2 \rceil} \in [0, \pi]$  for which  $R(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$  is a normal form of  $R$ , we define “redundant normal-form angles”  $\tilde{\theta}_i \in [0, \pi]$ ,  $1 \leq i \leq p$ , by

$$\tilde{\theta}_{2i-1} = \tilde{\theta}_{2i} = \theta_i, 1 \leq i \leq k = \lfloor \frac{p}{2} \rfloor; \quad \tilde{\theta}_p = 0 \text{ if } p = 2k + 1. \quad (7.9)$$

2. For any square matrix  $A$  we write  $E_\lambda(A)$  for the  $\lambda$ -eigenspace of  $A$ .

Note that (7.6) can now be written as

$$d_{SO(p)}(R, I)^2 = \frac{1}{2} \sum_{i=1}^p \tilde{\theta}_i^2. \quad (7.10)$$

## 7.2. Sign-change reducibility and distances between subspaces of $\mathbf{R}^p$

- Definition 7.2**
1. Call  $R \in SO(p)$  *sign-change reducible* if  $d_{SO(p)}(RI_\sigma, I) < d_{SO(p)}(R, I)$  for some  $\sigma \in \mathcal{I}_p^+$  (equivalently, if the pair  $(R, I)$  is sign-change reducible). Note that sign-change reducibility of the pair  $(U, V)$ , as previously defined in Definition 4.11, is equivalent to sign-change reducibility of  $V^{-1}U$ .
  2. For  $\sigma = (\sigma_1, \dots, \sigma_p) \in \mathcal{I}_p$ , define the *level* of  $\sigma$ , written  $\text{level}(\sigma)$ , to be  $\#\{i : \sigma_i = -1\}$ .
  3. For any involution  $R \in SO(p)$ , define the *level* of  $R$ , written  $\text{level}(R)$ , to be  $\dim(E_{-1}(R))$ . We write  $\text{Inv}(p)$  for the set of involutions in  $SO(p)$ , and for  $0 < m \leq p$  we write  $\text{Inv}_m(p)$  for the set of involutions in  $SO(p)$  of level  $m$ . Note that  $\dim(E_{-1}(R))$  is even for any  $R \in SO(p)$ , so  $\text{Inv}_m(p)$  is empty unless  $m$  is even and at least 2. Thus  $\text{Inv}(p) = \bigcup_{\text{even } m \geq 2} \text{Inv}_m(p)$  (a disjoint union).
  4. Let  $R \in SO(p)$  be an involution. We say that  $R$  is *reducible by a sign-change of level  $m$*  if there exists  $\sigma \in \mathcal{I}_p^+$  of level  $m$  such that  $d_{SO(p)}(RI_\sigma, I) < d_{SO(p)}(R, I)$ .

Observe that for non-identity  $\sigma \in \mathcal{I}_p^+$ , the matrix  $I_\sigma$  is an involution in  $SO(p)$ , and  $\text{level}(\sigma) = \text{level}(I_\sigma)$ . Also note that if  $R \in SO(p)$  is an involution of level  $m$ , then

$$d_{SO(p)}(R, I)^2 = \frac{m}{2} \pi^2. \quad (7.11)$$

**Remark 7.3** The space  $\text{Inv}(p)$  can be naturally identified with a disjoint union of Grassmannians, because an involution  $R \in SO(p)$  is completely determined by its  $(-1)$ -eigenspace  $E_{-1}(R)$ . Let  $\text{Gr}_m(\mathbf{R}^p)$  denote the Grassmannian of  $m$ -planes in  $\mathbf{R}^p$ , and for even  $m \in (0, p]$  define  $\Phi_{m,p} : \text{Gr}_m(\mathbf{R}^p) \rightarrow \text{Inv}_m(p)$  to be the map carrying  $W \in \text{Gr}_m(\mathbf{R}^p)$  to the involution in  $SO(p)$  whose  $(-1)$ -eigenspace is  $W$ . (Thus  $E_{-1}(R) = \Phi_{m,p}^{-1}(R)$  for all  $R \in \text{Inv}_m(p)$ .) Concretely, letting  $\pi_V : \mathbf{R}^p \rightarrow V$  denote orthogonal projection onto any subspace  $V$ , and letting  $P_V$  denote the matrix of  $\pi_V$  with respect to the standard basis of  $\mathbf{R}^p$ , the map  $\Phi_{m,p}$  is given by

$$\Phi_{m,p}(W) = P_{W^\perp} - P_W = 2P_{W^\perp} - I = I - 2P_W. \quad (7.12)$$

It is not hard to show that  $\text{Inv}_m(p)$  is a submanifold of  $SO(p)$  and that  $\Phi_{m,p}$  is a diffeomorphism from  $\text{Gr}_m(\mathbf{R}^p)$  to this submanifold.

As discussed in Section 4.3, a geodesically non-antipodal minimal pair in  $M$  uniquely determines an MSSR curve in  $\text{Sym}^+(p)$ . To understand whether the “Type II non-uniqueness” defined in Section 4.3 can occur, we need to know whether a geodesically antipodal pair in  $M$  can be minimal. A sufficient condition for any pair  $((U, D), (V, \Lambda))$  in  $M \times M$  to be *non-minimal* is that the pair  $(U, V) \in SO(p)$  be sign-change reducible. For  $p \leq 4$  one can show, without appealing to Proposition 7.5 below, that every involution in  $SO(p)$  is sign-change reducible. (This sign-change reducibility holds for trivial reasons for when  $p = 2$

; holds for slightly less trivial reasons for  $p = 3$  mentioned later in Remark 7.8; and can be shown to hold for  $p = 4$  using a quaternionic approach.) Potential Type II non-uniqueness complicates several aspects of the analysis of scaling-rotation distance and an associated metric (see [11]). Since sign-change reducibility of involutions rules out the possibility of Type II non-uniqueness, the  $p \leq 4$  sign-change reducibility motivates the following question:

**Question 7.4** *Let  $p \geq 2$ . Is every involution in  $SO(p)$  sign-change reducible?*

We shall see that the answer to Question 7.4 is “no” for  $p \geq 11$  (we do not know the answer for  $5 \leq p \leq 10$ ), but that for all  $p$ , involutions of high enough level are sign-change reducible, and by a sign-change of the same level:

**Proposition 7.5** *Let  $R \in SO(p)$  be an involution for which  $\text{level}(R) \geq \frac{1}{2}p$ . Then there exists  $\sigma \in \mathcal{I}_p^+$ , with  $\text{level}(\sigma) = \text{level}(R)$ , such that  $d_{SO(p)}(RI_\sigma, I) < d_{SO(p)}(R, I)$ .*

(Proofs of all results in this section are deferred to Section 7.3.)

Since  $\text{level}(R) = \dim(E_{-1}(R)) \geq 2$  for every involution  $R$ , Proposition 7.5 immediately establishes Proposition 4.13(a) and Corollary 4.14: for  $p \leq 4$ , all involutions are sign-change reducible, and hence all minimal pairs in  $M \times M$  are geodesically non-antipodal.

We shall see below (Proposition 7.6) that sign-change reducibility by a sign-change of the same level is equivalent to a statement purely about the geometry of Grassmannians. This geometric statement may be of interest independent of the context of this paper or the motivation for Question 7.4. We conjecture that the “same level” condition appearing in Proposition 7.5 is optimal (even without the “ $\text{level}(R) \geq \frac{1}{2}p$ ” restriction) in the sense that  $\min_{\sigma \in \mathcal{I}_p^+} \{d_{SO(p)}(RI_\sigma, I)\}$  is achieved by a sign-change matrix  $\sigma \in \mathcal{I}_p^+$  for which  $\text{level}(\sigma) = \text{level}(R)$ . If this is true, then the analysis of whether an involution  $R$  is sign-change reducible simplifies; we need only consider  $\sigma \in \mathcal{I}_p^+$  of the same level as  $R$ . This (potential) simplification is actually of greater value to us than knowing, for a given  $R \in \text{Inv}(p)$ , whether all minimizers of  $d_{SO(p)}(RI_\sigma, I)$  have the same level as  $R$ , so we state only the following weaker conjecture:

**Conjecture 7.6** *Let  $m \geq 2$  be even, and let  $R \in SO(p)$  be an involution of level  $m$ . If  $R$  is sign-change reducible, then it is reducible by a sign-change of level  $m$ .*

In Proposition 7.19 we will prove that this conjecture is true for the case  $m = 2$ .

The reason we expect that  $\min_{\sigma \in \mathcal{I}_p^+} \{d_{SO(p)}(RI_\sigma, I)\}$  is achieved by a  $\sigma$  for which  $\text{level}(\sigma) = \text{level}(R)$  is as follows. Every sign-change matrix  $I_{\sigma_1} \in \mathcal{I}_p^+$  is itself an involution, and satisfies

$$d_{SO(p)}(I_{\sigma_1} I_{\sigma_1}, I) = 0 < \min\{d_{SO(p)}(I_{\sigma_1} I_\sigma, I) : \sigma \in \mathcal{I}_p^+, \sigma \neq \sigma_1\}.$$

Thus for  $R \in SO(p)$  sufficiently close to  $I_{\sigma_1}$ , we have

$$d_{SO(p)}(RI_{\sigma_1}, I) < \min\{d_{SO(p)}(RI_\sigma, I) : \sigma \in \mathcal{I}_p^+, \sigma \neq \sigma_1\}.$$

The function carrying an involution in  $R \in SO(p)$  to  $\text{level}(R)$  is continuous, so for  $R \in \text{Inv}(p)$  sufficiently close to  $I_{\sigma_1}$  we also have  $\text{level}(R) = \text{level}(\sigma_1)$ . Hence for every  $R \in \text{Inv}(p)$  sufficiently close to a sign-change matrix,  $\min_{\sigma \in \mathcal{I}_p^+} \{d_{SO(p)}(RI_{\sigma}, I)\}$  is achieved by a sign-change matrix having the same level as  $R$ . It seems plausible that this remains true even without the “sufficiently close to a sign-change matrix” restriction.

As noted in Remark 7.3, for even  $m \geq 2$  the space  $\text{Inv}_m(p)$  is diffeomorphic to the Grassmannian  $\text{Gr}_m(\mathbf{R}^p)$ . This Grassmannian carries a Riemannian metric induced by Riemannian submersion from  $(SO(p), g_{SO(p)})$ . It is known that the associated squared geodesic-distance between two points  $W, Z \in \text{Gr}_m(\mathbf{R}^p)$  is, up to a constant factor, simply the sum of squares of the principal angles between the two  $m$ -planes  $W, Z$ .<sup>2</sup> Choosing the normalization in which the squared geodesic distance  $d_{Gr}(W, Z)^2$  equals the sum of squares of the principal angles (equation (7.15) below), we have the following:

**Proposition 7.7** *Let  $m, p$  be integers with  $m$  even and  $0 < m \leq p$ . Then the following two statements are equivalent:*

1. *Every involution  $R \in SO(p)$  of level  $m$  is sign-change reducible by a sign-change of level  $m$ .*
2. *For every  $W \in \text{Gr}_m(\mathbf{R}^p)$ , there exists a coordinate  $m$ -plane  $\mathbf{R}^J$  (see Notation 7.9) such that*

$$d_{Gr}(W, \mathbf{R}^J)^2 < \frac{m\pi^2}{8} . \quad (7.13)$$

In other words, the sign-change reducibility asserted in Statement 1 of the Proposition is equivalent to a statement purely about the geometry of Grassmannians (with the metric  $d_{Gr}$ ), namely that the coordinate  $m$ -planes in  $\mathbf{R}^p$  form a “lattice” of  $\binom{p}{m}$  points in  $\text{Gr}_m(\mathbf{R}^p)$  such that every point in  $\text{Gr}_m(\mathbf{R}^p)$  is within distance  $(m\pi^2/8)^{1/2}$  of some lattice-point. This gives us a geometric way to tackle Question 7.4, at least for sign-change reducibility of an involution  $R$  by a sign-change matrix of the same level. However, the authors do not know a formula for  $\min_{J \in \mathcal{J}_m} \{d_{Gr}(W, \mathbf{R}^J)\}$  for general  $W$ , or (more importantly)  $\max_{W \in \text{Gr}_p(\mathbf{R}^n)} \{\min_{J \in \mathcal{J}_m} \{d_{Gr}(W, \mathbf{R}^J)\}\}$ .

Proposition 7.7 is a consequence of a fact that we prove later as Corollary 7.14: the diffeomorphism  $\Phi_{m,p}$  defined in (7.12) is actually a metric-space isometry up to a constant factor. Corollary 7.14 can be proven by purely Riemannian methods, but the proof we give is independent in the sense that it does not make any use of a Riemannian metric on  $\text{Gr}_m(\mathbf{R}^p)$ ; see Remark 7.15.

Note that Proposition 7.5 asserts that statement 1 of Proposition 7.7 is true whenever  $m \geq \frac{p}{2}$ . To put the number  $\frac{m}{8}\pi^2$  and the relation between  $m$  and  $\frac{p}{2}$  in perspective, note that the squared diameter of  $\text{Gr}_m(\mathbf{R}^p)$  is  $\min\{m, p-m\}\frac{\pi^2}{4}$ . So for  $m \leq \frac{p}{2}$ , (7.13) is equivalent to

$$d_{Gr}(W, \mathbf{R}^J)^2 < \frac{1}{2} \text{diam}(\text{Gr}_m(\mathbf{R}^p))^2. \quad (7.14)$$

<sup>2</sup>This fact follows from Wong’s results on geodesics in [19], and has been cited elsewhere in the literature (e.g. [7, p. 337]), though the explicit statement does not appear in [19].

For  $m > \frac{p}{2}$ , the right-hand side of (7.13) is a greater fraction of  $\text{diam}(\text{Gr}_m(\mathbf{R}^p))^2$ , so it is "easier" for statement 2 of Proposition 7.7 to be true for  $m > \frac{p}{2}$  than for  $m < \frac{p}{2}$ .

**Remark 7.8** It is relatively easy to show that for any involution  $R$ , there exists  $\sigma$  for which  $RI_\sigma$  is not an involution. For  $p = 2, 3$ , we have  $d_{SO(p)}(I, R) \leq \pi$  for every  $R \in SO(p)$ , and  $d_{SO(p)}(I, R) = \pi$  for every involution  $R$ , so any non-involution is closer to the identity than is any involution. Hence for these values of  $p$ , Proposition 7.7 is easy to prove. However, for  $p \geq 4$ , given an involution  $R$  and a  $\sigma \in \mathcal{I}_p^+$  for which  $RI_\sigma$  is not an involution, (7.8) shows that we cannot immediately deduce that  $d_{SO(p)}(I, RI_\sigma) < d_{SO(p)}(I, R)$ .

### 7.3. Main results

In this subsection, after the technical Lemma 7.10, we establish the results alluded to earlier that may be of interest outside the context of this paper: the half-angle formula (7.39) and its generalization (7.46) relating the principal angles between the  $(-1)$ -eigenspaces of two involutions to the normal-formal angles of the product of the involutions, and the "non-Riemannian" proof of the isometric correspondence between  $\text{Inv}_m(p)$  and  $\text{Gr}_m(\mathbf{R}^p)$  (Corollary 7.14). We also prove that Conjecture 7.6 is true for the case  $m = 2$  (Corollary 7.19). Using these facts, we prove the results stated in Section 7.2, as well as Proposition 4.15. (The latter is proven in stages, with part (a) following from Proposition 7.5, and part (b) following from Proposition 7.19, Corollary 7.19, and Examples 7.20 and 7.21.)

We start with some notation.

#### Notation 7.9

1. For  $1 \leq i \leq p$  let  $\mathbf{e}_i$  denote the  $i^{\text{th}}$  standard basis vector of  $\mathbf{R}^p$ .
2. For  $0 \leq m \leq p$ , let  $\mathcal{J}_{m,p}$  denote the collection of  $m$ -element subsets of  $\{1, \dots, p\}$ .
  - (a) For  $0 \leq m \leq p$  and  $J \in \mathcal{J}_{m,p}$ , define  $\sigma^J = (\sigma_1, \dots, \sigma_p) \in \mathcal{I}_p$  by  $\sigma_i = -1$  for  $i \in J$  and  $\sigma_i = 1$  for  $i \notin J$ . Similarly, for  $\sigma = (\sigma_1, \dots, \sigma_p) \in \mathcal{I}_p$ , define  $J^\sigma = \{i \in \{1, \dots, p\} : \sigma_i = -1\}$ . (The maps  $J \mapsto \sigma^J$  and  $\sigma \mapsto J^\sigma$  are inverse to each other.)
  - (b) If  $1 \leq m \leq p$  and  $J = \{i_1, \dots, i_m\} \in \mathcal{J}_{m,p}$ , with  $i_1 < i_2 < \dots < i_m$ , let  $\mathbf{E}_J$  denote the  $p \times m$  matrix whose  $k^{\text{th}}$  column is  $\mathbf{e}_{i_k}$ ,  $1 \leq k \leq m$ .
  - (c) For  $0 \leq m \leq p$  and  $J \in \mathcal{J}_{m,p}$ , define  $\mathbf{R}^J = \{(x^1, x^2, \dots, x^p) \in \mathbf{R}^p : x^i = 0 \text{ if } i \notin J\}$ .

The collection  $\{\mathbf{R}^J : J \in \mathcal{J}_{m,p}\}$  is the set of "coordinate  $m$ -planes" in  $\mathbf{R}^p$ .

3. For any  $J \subset \{1, \dots, p\}$ , let  $J'$  denote the complement of  $J$  in  $\{1, \dots, p\}$ .
4. For  $m_1, m_2 \in \{1, 2, \dots, p\}$ ,  $W \in \text{Gr}_{m_1}(\mathbf{R}^p)$ ,  $Z \in \text{Gr}_{m_2}(\mathbf{R}^p)$ , and  $J \in \mathcal{J}_{m_1,p}$ , writing  $m = \min\{m_1, m_2\}$ ,
  - (a) let  $\phi_1(W, Z), \dots, \phi_m(W, Z)$ , denote the principal angles between the  $m_1$ -plane  $W$  and the  $m_2$ -plane  $Z$  (see [9, Section 12.4.3]), and

- (b) let  $\phi_{J,i}(W) = \phi_i(W, \mathbf{R}^J)$ ,  $1 \leq i \leq m_1$ .
5. For  $1 \leq m \leq p$  define  $d_{Gr} : \text{Gr}_m(\mathbf{R}^p) \times \text{Gr}_m(\mathbf{R}^p) \rightarrow \mathbf{R}$  by

$$d_{Gr}(W, Z) = \left( \sum_{i=1}^m \phi_i(W, Z)^2 \right)^{1/2}. \quad (7.15)$$

As noted earlier,  $d_{Gr}$  is the distance-function defined by the standard  $SO(p)$ -invariant Riemannian metric on  $\text{Gr}_m(\mathbf{R}^p)$  (up to a constant factor).

The following technical lemma is our tool for comparing  $d_{SO(p)}(RI_\sigma, I)$  to  $d_{SO(p)}(R, I)$  for an involution  $R$  and sign-change matrix  $I_\sigma$ , and also leads to the half-angle formula and to Corollary 7.14.

**Lemma 7.10** *Let  $R \in SO(p)$  be an involution, let  $\sigma \in \mathcal{I}_p^+$ , assume  $0 < m_\sigma := \text{level}(\sigma) < p$ , and let  $J = J^\sigma$  (see Notation 7.9). Viewing  $\mathbf{R}^p$  as  $\mathbf{R}^{J'} \oplus \mathbf{R}^J$ , below we write every  $p \times p$  matrix in the block form  $\begin{bmatrix} A_1 & A_2 \\ A_3 & A_4 \end{bmatrix}$ , where  $A_1$  is  $(p - m_\sigma) \times (p - m_\sigma)$ ,  $A_2$  is  $(p - m_\sigma) \times m_\sigma$ ,  $A_3$  is  $m_\sigma \times (p - m_\sigma)$ , and  $A_4$  is  $m_\sigma \times m_\sigma$ . Then:*

(i) *In this block form,*

$$R = \begin{bmatrix} R_1 & R_2 \\ R_2^T & R_4 \end{bmatrix}, \quad (7.16)$$

where  $R_1$  is a symmetric  $(p - m_\sigma) \times (p - m_\sigma)$  matrix,  $R_4$  is a symmetric  $m_\sigma \times m_\sigma$  matrix, and  $R_2$  is  $(p - m_\sigma) \times m_\sigma$ .

(ii) *In the same block form,*

$$(RI_\sigma)_{\text{sym}} = \frac{1}{2}(RI_\sigma + I_\sigma R) = \begin{bmatrix} R_1 & 0 \\ 0 & -R_4 \end{bmatrix}. \quad (7.17)$$

(iii) *All eigenvalues of  $R_1$  and  $R_4$  lie in the interval  $[-1, 1]$ .*

(iv) *For every  $\lambda \in (-1, 1)$ , if  $\lambda$  is an eigenvalue of  $R_1$  (respectively,  $R_4$ ), then  $-\lambda$  is an eigenvalue of  $R_4$  (resp.  $R_1$ ) with the same multiplicity.*

(v) *Let  $l$  denote the number of eigenvalues of  $R_1$ , counted with multiplicity, lying in the interval  $(-1, 1)$ . Then  $l$  is also the number of eigenvalues of  $R_4$ , counted with multiplicity, lying in  $(-1, 1)$ , and  $l \leq \min\{m_\sigma, p - m_\sigma\}$ .*

(vi) *The inclusion map  $\mathbf{R}^{J'} \rightarrow \mathbf{R}^p$  defined by  $v \mapsto \begin{bmatrix} v \\ 0 \end{bmatrix}$  restricts to isomorphisms  $E_{\pm 1}(R_1) \rightarrow E_{\pm 1}(R) \cap \mathbf{R}^{J'}$ . Similarly the inclusion map  $\mathbf{R}^J \rightarrow \mathbf{R}^p$  defined by  $w \mapsto \begin{bmatrix} 0 \\ w \end{bmatrix}$  restricts to isomorphisms  $E_{\pm 1}(R_4) \rightarrow E_{\pm 1}(R) \cap \mathbf{R}^J$ .*

(vii) *Let  $l_- = \dim(E_1(R) \cap \mathbf{R}^J)$ ,  $l_+ = \dim(E_{-1}(R) \cap \mathbf{R}^{J'})$ .<sup>3</sup> Then  $\dim(E_1(R_4)) = l_-$  and  $\dim(E_{-1}(R_1)) = l_+$ . (Thus  $l_- + l_+$  is the multiplicity of*

<sup>3</sup>The  $\pm$  subscripts are chosen according to the eigenspaces of  $I_\sigma$  rather than  $R$ :  $\mathbf{R}^J = E_{-1}(I_\sigma)$ ,  $\mathbf{R}^{J'} = E_1(I_\sigma)$ .

$-1$  as an eigenvalue of  $(RI_\sigma)_{\text{sym}}$  in (7.17), hence of  $RI_\sigma$  itself, and therefore yields a lower bound on  $d_{SO(p)}(RI_\sigma, I)$ .) Furthermore,

$$l_- \geq \text{level}(\sigma) - \text{level}(R) \quad \text{and} \quad l_+ \geq \text{level}(R) - \text{level}(\sigma), \quad (7.18)$$

and

$$l_- - l_+ = \text{level}(\sigma) - \text{level}(R). \quad (7.19)$$

(viii) There exist an orthonormal  $R_1$ -eigenbasis  $\{v_i\}_{i=1}^{p-m_\sigma}$  of  $\mathbf{R}^{p-m_\sigma}$  (i.e. an orthonormal basis of  $\mathbf{R}^{p-m_\sigma}$  consisting of eigenvectors of  $R_1$ ) and an  $R_4$ -eigenbasis  $\{w_i\}_{i=1}^{m_\sigma}$  of  $\mathbf{R}^{m_\sigma}$ . For any such bases  $\{v_i\}$  of  $\mathbf{R}^{p-m_\sigma}$ ,  $\{w_i\}$  of  $\mathbf{R}^{m_\sigma}$ , let  $\{\lambda'_i\}, \{\lambda_i\}$  be the corresponding eigenvalues (i.e.  $R_1 v_i = \lambda'_i v_i$  and  $R_4 w_i = \lambda_i w_i$ ), and define

$$\mathbf{v}_i = \begin{cases} \begin{bmatrix} v_i \\ \frac{1}{1+\lambda'_i} R_2^T v_i \end{bmatrix}, & 1 \leq i \leq p-m_\sigma, \lambda'_i \neq -1, \\ \begin{bmatrix} v_i \\ 0 \end{bmatrix}, & 1 \leq i \leq p-m_\sigma, \lambda'_i = -1, \end{cases} \quad (7.20)$$

$$\mathbf{w}_i = \begin{cases} \begin{bmatrix} \frac{-1}{1-\lambda_i} R_2 w_i \\ w_i \end{bmatrix}, & 1 \leq i \leq m_\sigma, \lambda_i \neq 1, \\ \begin{bmatrix} 0 \\ w_i \end{bmatrix}, & 1 \leq i \leq m_\sigma, \lambda_i = 1. \end{cases} \quad (7.21)$$

Then

$$\left\{ \sqrt{\frac{1+\lambda'_i}{2}} \mathbf{v}_i : 1 \leq i \leq p-m_\sigma, \lambda'_i \neq -1 \right\} \cup \{ \mathbf{w}_i : 1 \leq i \leq m_\sigma, \lambda_i = 1 \} \quad (7.22)$$

(ordered arbitrarily) is an orthonormal basis of  $E_1(R)$ , and the set

$$\left\{ \sqrt{\frac{1-\lambda_i}{2}} \mathbf{w}_i : 1 \leq i \leq m_\sigma, \lambda_i \neq 1 \right\} \cup \{ \mathbf{v}_i : 1 \leq i \leq p-m_\sigma, \lambda'_i = -1 \} \quad (7.23)$$

(ordered arbitrarily) is an orthonormal basis of  $E_{-1}(R)$ . Note that the cardinality of the second set in (7.22) (respectively (7.23)) is  $l_-$  (resp.  $l_+$ ).

**Proof:** To simplify notation in this proof, we let  $m = m_\sigma$ .

Since  $R \in SO(p)$  is an involution,  $R = R^{-1} = R^T$ . Hence  $R$  is symmetric, implying assertion (i), and  $\mathbf{R}^p$  is the orthogonal direct sum of  $E_1(R)$  and  $E_{-1}(R)$  (since the only possible eigenvalues of an involution are  $\pm 1$ ).

For (ii), observe that in the block-form decomposition we are using,

$$I_\sigma = \begin{bmatrix} I_{(p-m) \times (p-m)} & 0 \\ 0 & -I_{m \times m} \end{bmatrix}.$$

A simple calculation then yields (7.17).

Next, because  $R^2 = I$ , we have the following relations:

$$R_1^2 + R_2 R_2^T = I_{(p-m) \times (p-m)}, \quad (7.24)$$

$$R_1 R_2 + R_2 R_4 = 0_{(p-m) \times m}, \quad (7.25)$$

$$R_2^T R_1 + R_4 R_2^T = 0_{m \times (p-m)}, \quad (7.26)$$

$$R_4^2 + R_2^T R_2 = I_{m \times m}. \quad (7.27)$$

From (7.24) and (7.27), for any  $v \in \mathbf{R}^{p-m}, w \in \mathbf{R}^m$ , we have

$$\|R_1 v\|^2 + \|R_2^T v\|^2 = \|v\|^2, \quad (7.28)$$

$$\|R_4 w\|^2 + \|R_2 w\|^2 = \|w\|^2. \quad (7.29)$$

It follows from (7.28)–(7.29) that if  $\lambda$  is an eigenvalue of  $R_1$  or  $R_4$ , then  $|\lambda| \leq 1$ , yielding (iii).

To obtain (iv), consider the operators  $L : \mathbf{R}^m \rightarrow \mathbf{R}^{p-m}$  and  $L^* : \mathbf{R}^{p-m} \rightarrow \mathbf{R}^m$  defined by  $L(w) = R_2 w$  and  $L^*(v) = R_2^T v$ . Suppose that  $R_1$  has an eigenvalue  $\lambda$  with  $|\lambda| < 1$ , and let  $0 \neq v \in E_\lambda(R_1)$ . Let  $w = R_2^T v$ ; note that (7.28) implies  $w \neq 0$ . Using (7.26),

$$R_4 w = R_4 R_2^T v = -R_2^T R_1 v = -R_2^T \lambda v = -\lambda w.$$

Hence  $L^*$  maps  $E_\lambda(R_1)$  injectively to  $E_{-\lambda}(R_4)$ . Similarly, if  $R_4$  has an eigenvalue  $-\lambda$  with  $|\lambda| < 1$ , and  $L^*$  maps  $E_{-\lambda}(R_4)$  injectively to  $E_\lambda(R_1)$ .

It follows that, for any  $\lambda \in \mathbf{R}$  with  $|\lambda| < 1$ ,  $\lambda$  is an eigenvalue of  $R_1$  if and only if  $-\lambda$  is an eigenvalue of  $R_4$ , and that the maps

$$L^*|_{E_\lambda(R_1)} : E_\lambda(R_1) \rightarrow E_{-\lambda}(R_4) = E_\lambda(-R_4), \quad (7.30)$$

$$L|_{E_\lambda(-R_4)} : E_\lambda(-R_4) = E_{-\lambda}(R_4) \rightarrow E_\lambda(R_1) \quad (7.31)$$

are isomorphisms. This establishes (iv). Statement (v) is an immediate corollary of (iv).

For (vi), let  $\iota : \mathbf{R}^{J'} \rightarrow \mathbf{R}^p$  be the first inclusion map in the lemma. Note that  $R \begin{bmatrix} v \\ 0 \end{bmatrix} = \begin{bmatrix} R_1 v \\ R_2^T v \end{bmatrix}$ . If  $v \in E_\lambda(R_1)$  with  $\lambda = \pm 1$ , equation (7.28) implies that  $R_2^T v = 0$ , hence that  $R\iota(v) = \lambda\iota(v)$ . Conversely, if  $R\iota(v) = \lambda\iota(v)$ , then  $R_1 v = \lambda v$  (and  $R_2^T v = 0$ ). Hence  $\iota$  carries  $E_\lambda(R_1)$  isomorphically to  $E_\lambda(R) \cap \mathbf{R}^{J'}$ . The argument for the inclusion map  $\mathbf{R}^J \rightarrow \mathbf{R}^p$  is essentially identical. This establishes (vi).

Part (vi) implies that  $\dim(E_1(R_4)) = \dim(E_1(R) \cap \mathbf{R}^J) = l_-$  and that  $\dim(E_{-1}(R_1)) = \dim(E_{-1}(R) \cap \mathbf{R}^{J'}) = l_+$ , the first assertion in (vii). To obtain (7.18)–(7.19), note that for any subspaces  $V, W$  of  $\mathbf{R}^p$ , we have

$$\dim(V^\perp \cap W) - \dim(V \cap W^\perp) = \dim(W) - \dim(V). \quad (7.32)$$

(The proof of (7.32) is straightforward linear algebra.) Applying this to the case  $V = E_{-1}(R), V^\perp = E_1(R), W = E_{-1}(I_\sigma) = \mathbf{R}^J, W^\perp = E_1(I_\sigma) = \mathbf{R}^{J'}$ ,



we have  $l_- = \dim(V^\perp \cap W)$  and  $l_+ = \dim(V \cap W^\perp)$ , so (7.19) follows from (7.32). The inequalities in (7.18) follow directly from (7.19).

(viii) Since  $R_1$  (respectively  $R_4$ ) is symmetric, an orthonormal  $R_1$ -eigenbasis  $\{v_i\}$  of  $\mathbf{R}^{p-m}$  (resp., orthonormal  $R_4$ -eigenbasis  $\{w_i\}$  of  $\mathbf{R}^m$ ) exists. Select such eigenbases, and let  $\{\lambda_i\}$ ,  $\{\lambda'_i\}$  be eigenvalues as defined in the Lemma. Note that the second set in (7.22) is a basis of  $E_1(R_4)$ , which by (vi) is isomorphic to  $E_1(R) \cap \mathbf{R}^J$ . Hence the cardinality of this set is  $\dim(E_1(R) \cap \mathbf{R}^J)$ , i.e.  $l_-$ . Similarly, the second set in (7.23) is a basis of  $E_{-1}(R_1)$  and has cardinality  $l_+$ .

Without loss of generality, we may assume that the eigenvectors  $v_i$  with eigenvalue  $-1$ , if any, are the last  $l_+$ , and that the eigenvectors  $w_i$  with eigenvalue  $1$ , if any, are the last  $l_-$ . Using (7.27), for  $1 \leq i \leq m$  we have  $R_2^T R_2 w_i = (1 - \lambda_i^2)w_i$ , while using (7.25) we find  $R_1 R_2 w_i = -\lambda_i R_2 w_i$ . Then, using (7.16), a simple calculation shows that  $R w_i = -w_i$ . Hence  $w_i \in E_{-1}(R)$  for  $1 \leq i \leq m - l_-$ , while from part (vi),  $v_i \in E_{-1}(R)$  for  $p - m - l_+ < i \leq p - m$ .

Let  $\langle \cdot, \cdot \rangle$  denote the standard inner product on  $\mathbf{R}^n$  for any  $n$ . As seen in the proof of part (vi),  $v \in E_{-1}(R_1)$  implies  $R_2^T v = 0$ . Hence for  $p - m - l_+ < i \leq p - m$  and  $1 \leq j \leq m - l_-$ ,  $\langle v_i, w_j \rangle \propto \langle v_i, R_2 w_j \rangle = \langle R_2^T v_i, w_j \rangle = 0$ , while for  $p - m - l_+ < i, j \leq p - m$  we have  $\langle v_i, v_j \rangle = \langle v_i, v_j \rangle = \delta_{ij}$ . Finally, for  $i, j \leq m - l_-$ , using the fact that  $\langle R_2 w_i, R_2 w_j \rangle = \langle w_i, R_2^T R_2 w_j \rangle = \langle w_i, (1 - \lambda_i^2)w_j \rangle$ , a simple computation yields  $\langle w_i, w_j \rangle = \frac{2}{1 - \lambda_i^2} \delta_{ij}$ . Thus  $\{\sqrt{\frac{1 - \lambda_i^2}{2}} w_i : 1 \leq i \leq m - l_-\} \cup \{v_i : p - m - l_+ < i \leq p - m\}$  is an orthonormal subset of  $E_{-1}(R)$ . Using (7.19), the cardinality of this subset is  $m - l_- + l_+ = \text{level}(\sigma) - (\text{level}(\sigma) - \text{level}(R)) = \text{level}(R) = \dim(E_{-1}(R))$ . Hence (7.23) is an orthonormal basis of  $E_{-1}(R)$ .

The proof that (7.22) is an orthonormal basis of  $E_1(R)$  is similar.  $\blacksquare$

**Corollary 7.11** *Hypotheses and notation as in Lemma 7.10. Let  $l_+ = \dim(E_{-1}(R_1))$  and  $l_- = \dim(E_1(R_4))$  (as in Lemma 7.10(vii)). In addition let  $\{\theta_i \in [0, \pi]\}_{i=1}^{\lfloor p/2 \rfloor}$  be angles for which  $R(\theta_1, \dots, \theta_{\lfloor p/2 \rfloor})$  is a normal form of  $RI_\sigma$ , and let  $\{\tilde{\theta}_i\}_{i=1}^p$  be as defined in (7.9). Let  $J_* = \{j \in J : 0 < \tilde{\theta}_j < \pi\}$ . Then  $|J_*| \leq \min\{m_\sigma, p - m_\sigma\}$ , and*

$$d_{SO(p)}(RI_\sigma, I)^2 = \frac{1}{2}(l_+ + l_-)\pi^2 + \sum_{j \in J_*} \tilde{\theta}_j^2. \quad (7.33)$$

If  $\text{level}(\sigma) = \text{level}(R)$ , then

$$d_{SO(p)}(RI_\sigma, I)^2 = l_- \pi^2 + \sum_{j \in J_*} \tilde{\theta}_j^2 = \sum_{j \in J} \tilde{\theta}_j^2. \quad (7.34)$$

**Proof:** Let  $\beta' : J' \rightarrow \{1, \dots, p - m_\sigma\}$ ,  $\beta : J \rightarrow \{1, \dots, m_\sigma\}$ , be order-preserving bijections. By (7.7), the eigenvalues of  $(RI_\sigma)_{\text{sym}}$ , counted with multiplicity, are  $\{\cos \tilde{\theta}_i\}_{i=1}^p$ . But from Lemma 7.10(ii), we can read off the eigenvalues of  $(RI_\sigma)_{\text{sym}}$  from (7.17); they are  $\lambda'_1, \dots, \lambda'_{p-m_\sigma}, -\lambda_1, \dots, -\lambda_{m_\sigma}$  (ordered arbitrarily). Thus, reordering the  $\lambda'_j$  and the  $\lambda_j$  appropriately, for  $1 \leq j \leq p$  we

have

$$\cos \tilde{\theta}_j = \begin{cases} \lambda'_{\beta'(j)} & \text{if } j \in J', \\ -\lambda_{\beta(j)} & \text{if } j \in J. \end{cases} \quad (7.35)$$

Define  $J_* = \{j \in J : \lambda_{\beta(j)} \neq \pm 1\}$ . Observe that  $J_*$  can also be characterized as  $\{j \in J : \lambda_{\beta(j)} \neq \pm 1\}$ . Similarly, define  $J'_* = \{j \in J' : \lambda'_{\beta'(j)} \neq \pm 1\} = \{j \in J' : 0 < \tilde{\theta}_j < \pi\}$ . By part (v) of Lemma 7.10,  $|J'_*| = |J_*| = l \leq \min\{m_\sigma, p - m_\sigma\}$ , and by part (iv) of the Lemma there is a bijection  $b : J_* \rightarrow J'_*$  such that  $-\lambda_j = \lambda'_{b(j)}$  for all  $j \in J_*$ . Hence

$$\tilde{\theta}_j = \begin{cases} \cos^{-1} \lambda'_{\beta'(j)} & \text{if } j \in J'_*, \\ \cos^{-1} \lambda'_{b(\beta(j))} & \text{if } j \in J_*, \\ 0 \text{ or } \pi & \text{otherwise.} \end{cases} \quad (7.36)$$

In particular,

$$\sum_{j \in J_*} \tilde{\theta}_j^2 = \sum_{j \in J'_*} \tilde{\theta}_j^2. \quad (7.37)$$

Next, note that

$$\sum_{j \in J' \setminus J'_*} \tilde{\theta}_j^2 = \sum_{\{j \in J' : \tilde{\theta}_j = \pi\}} \tilde{\theta}_j^2 = \#\{j \in J' : \lambda'_{\beta'(j)} = -1\} \pi^2 = \dim(E_{-1}(R_1)) \pi^2 = l_+ \pi^2, \quad (7.38)$$

and similarly  $\sum_{j \in J \setminus J_*} \tilde{\theta}_j^2 = l_- \pi^2$ . From (7.10) we therefore have

$$\begin{aligned} d_{SO(p)}(RI_\sigma, I)^2 &= \frac{1}{2} \left\{ \sum_{j \in J' \setminus J'_*} \tilde{\theta}_j^2 + \sum_{j \in J \setminus J_*} \tilde{\theta}_j^2 + \sum_{j \in J'_*} \tilde{\theta}_j^2 + \sum_{j \in J_*} \tilde{\theta}_j^2 \right\} \\ &= \frac{1}{2} \left\{ l_+ \pi^2 + l_- \pi^2 + 2 \sum_{j \in J_*} \tilde{\theta}_j^2 \right\}, \end{aligned}$$

establishing (7.33).

If  $\text{level}(\sigma) = \text{level}(R)$ , then equation (7.19) implies that  $l_+ = l_-$ , so (7.33) implies the first equality in (7.34). For the second equality, observe that  $j \in J \setminus J_*$  if and only if  $\tilde{\theta}_j$  is 0 or  $\pi$ . The number of  $j$ 's in  $J$  for which  $\tilde{\theta}_j = \pi$  is exactly  $l_-$ , while the  $j$ 's in  $J$  for which  $\tilde{\theta}_j = 0$  have no effect on  $\sum_{j \in J} \tilde{\theta}_j^2$ . Hence the second equality in (7.34) holds.  $\blacksquare$

For  $R \in \text{Inv}(p)$  and  $\sigma \in \mathcal{I}_p^+$ , the following corollary relates the normal-form angles of  $RI_\sigma$  to the principal angles between  $E_{-1}(R)$  and  $\mathbf{R}^J = E_{-1}(I_\sigma)$ . When  $\text{level}(R) = \text{level}(\sigma) = m$ , this leads to a simple relation between  $d_{SO(p)}(RI_\sigma, I)$  and distance in  $\text{Gr}_m(\mathbf{R}^p)$  between these  $(-1)$ -eigenspaces.

**Corollary 7.12** *Hypotheses and notation as in Lemma 7.10, except that we additionally write  $m_R := \text{level}(R)$  and  $m = \min\{m_\sigma, m_R\}$ . Let  $\{\theta_i \in [0, \pi]\}_{i=1}^{\lceil p/2 \rceil}$*

be angles for which  $R(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$  is a normal form of  $RI_\sigma$ , let  $\{\tilde{\theta}_i\}_{i=1}^p$  be as defined in (7.9), let the elements of  $J$  be  $i_1 < i_2 < \dots < i_{m_\sigma}$ , and let  $\phi_{J,j} = \phi_{J,j}(E_{-1}(R))$ ,  $1 \leq j \leq m$ . Then:

(i) Up to ordering,

$$\phi_{J,j} = \frac{\tilde{\theta}_{i_j}}{2}, \quad 1 \leq j \leq m. \quad (7.39)$$

(ii) If  $m_\sigma = m_R$  then

$$d_{SO(p)}(RI_\sigma, I) = 2d_{Gr}(E_{-1}(R), \mathbf{R}^J). \quad (7.40)$$

**Proof:** (i). Let  $\widetilde{W}$  be the  $p \times m_R$  matrix formed by the columns of the basis (7.23) of  $E_{-1}(R)$ , with the elements of the first set in (7.23) comprising the first  $m_\sigma - l_-$  columns, and the elements of the second set comprising the last  $l_+$  columns. (Here  $l_\pm$  are defined as in Lemma 7.10(vii).) Without loss of generality we order the  $R_4$ -eigenvectors  $w_i$  such that the first  $m_\sigma - l_-$  are the ones for which  $\lambda_i \neq 1$ .

Since the columns of  $\widetilde{W}$  form an orthonormal basis of  $E_{-1}(R)$ , the numbers  $\{\cos \phi_{J,i}\}_{i=1}^m$  are the singular values of the  $m_R \times m_\sigma$  matrix  $\widetilde{W}^T \mathbf{E}_J$ . (This is true whether  $m_R \leq m_\sigma$  or  $m_R > m_\sigma$ .) But, relative to the block-decomposition of matrices used in Lemma 7.10, the upper  $(p - m_\sigma) \times m_\sigma$  block of  $\mathbf{E}_J$  is 0, and the lower  $m_\sigma \times m_\sigma$  block is  $I_{m_\sigma \times m_\sigma}$ . Hence, writing  $\widetilde{W}_*$  for the  $m_\sigma \times (m_\sigma - l_-)$  matrix formed by the last  $m_\sigma$  rows of the first  $m_\sigma - l_-$  columns of  $\widetilde{W}$ , and noting that  $m_\sigma - l_- = m_R - l_+$  (by (7.19)), we have  $\widetilde{W}^T \mathbf{E}_J = \begin{bmatrix} \widetilde{W}_*^T \\ 0_{l_+ \times m_\sigma} \end{bmatrix}$ , where the  $i^{\text{th}}$  row of the  $(m_\sigma - l_-) \times (p - m_\sigma)$  matrix  $\widetilde{W}_*^T$  is a multiple of  $w_i^T$ . Hence for  $i, j \leq m_\sigma - l_- = m_R - l_+$ ,

$$\left( (\widetilde{W}^T \mathbf{E}_J)(\widetilde{W}^T \mathbf{E}_J)^T \right)_{ij} = \sqrt{\frac{1 - \lambda_i}{2}} \sqrt{\frac{1 - \lambda_j}{2}} \langle w_i, w_j \rangle = \frac{1 - \lambda_j}{2} \delta_{ij}, \quad (7.41)$$

and all other entries of the  $m_R \times m_R$  matrix  $\widetilde{W}^T \mathbf{E}_J (\widetilde{W}^T \mathbf{E}_J)^T$  are 0. But for  $m_\sigma - l_- < i \leq m_\sigma$ , we have  $\lambda_i = 1$ , so  $\left( (\widetilde{W}^T \mathbf{E}_J)(\widetilde{W}^T \mathbf{E}_J)^T \right)_{ij} = \frac{1 - \lambda_j}{2} \delta_{ij}$  for all  $i, j \leq m = \min\{m_R, m_\sigma\}$ . Thus the upper left-hand  $m \times m$  block of  $(\widetilde{W}^T \mathbf{E}_J)(\widetilde{W}^T \mathbf{E}_J)^T$  (the entire  $m_R \times m_R$  matrix if  $m_R \leq m_\sigma$ ) is  $\text{diag}(\frac{1 - \lambda_1}{2}, \dots, \frac{1 - \lambda_m}{2})$ , so the numbers  $\sqrt{\frac{1 - \lambda_j}{2}}$ ,  $1 \leq j \leq m$ , are the singular values of  $\widetilde{W}^T \mathbf{E}_J$ . Thus, up to ordering, the principal angles  $\{\phi_{J,i}\}$  are given by

$$\cos \phi_{J,j} = \sqrt{\frac{1 - \lambda_j}{2}}, \quad 1 \leq j \leq m. \quad (7.42)$$

The bijection  $\beta : J \rightarrow \{1, \dots, m_\sigma\}$  used in the proof of Corollary 7.11 is simply the inverse of the map  $j \mapsto i_j$ . Thus from (7.35), we have

$$-\lambda_j = \cos \tilde{\theta}_{i_j}, \quad 1 \leq j \leq m_\sigma. \quad (7.43)$$

Combining (7.42) with (7.43),

$$\cos \phi_{J,j} = \sqrt{\frac{1 + \cos \tilde{\theta}_{i_j}}{2}} = \cos \frac{\tilde{\theta}_{i_j}}{2}. \quad (7.44)$$

But  $\tilde{\theta}_{i_j} \in [0, \pi]$ , so both  $\phi_{J,j}$  and  $\frac{\tilde{\theta}_{i_j}}{2}$  lie in  $[0, \frac{\pi}{2}]$ . Hence (7.44) implies that  $\phi_{J,j} = \tilde{\theta}_{i_j}/2$ ,  $1 \leq j \leq m$ .

(ii) Assume  $m_\sigma = m_R$ ; then both equal  $m$ . Corollary 7.11 then implies that

$$d_{SO(p)}(RI_\sigma, I)^2 = \sum_{i=1}^m \tilde{\theta}_{i_j}^2. \quad (7.45)$$

But from part (i) we have  $\tilde{\theta}_{i_j} = 2\phi_{J,j}$  for  $1 \leq j \leq m$ , so, using (7.34),  $d_{SO(p)}(RI_\sigma, I)^2 = 4d_{Gr}(E_{-1}(R), \mathbf{R}^J)^2$ , implying (7.40). ■

**Corollary 7.13** *Let  $R_1, R_2$  be involutions in  $SO(p)$ . For  $i = 1, 2$  let  $m_i = \dim(E_{-1}(R_i))$ , and let  $m = \min\{m_1, m_2\}$ . Let  $\{\theta_i \in [0, \pi]\}_{i=1}^{\lceil p/2 \rceil}$  be angles for which  $R(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$  is a normal form of the product  $R_1 R_2$ , and let  $\{\tilde{\theta}_i\}_{i=1}^p$  be as defined in (7.9). Then for some injective map  $\iota : \{1, 2, \dots, m\} \rightarrow \{1, 2, \dots, p\}$ , the principal angles between  $E_{-1}(R_1)$  and  $E_{-1}(R_2)$  satisfy*

$$\phi_j(E_{-1}(R_1), E_{-1}(R_2)) = \frac{\tilde{\theta}_{\iota(j)}}{2}, \quad 1 \leq j \leq m. \quad (7.46)$$

For every  $i \notin \text{range}(\iota)$ , the angle  $\tilde{\theta}_i$  is either 0 or  $\pi$ .

**Proof:** Let  $U \in O(p)$  and let  $T_U : \mathbf{R}^p \rightarrow \mathbf{R}^p$  be the corresponding orthogonal transformation. For any even  $m' > 0$  and any  $R \in \text{Inv}_{m'}(p)$ , we have

$$E_{-1}(URU^{-1}) = T_U(E_{-1}(R)). \quad (7.47)$$

Now let  $T : \mathbf{R}^p \rightarrow \mathbf{R}^p$  be an orthogonal transformation carrying  $E_{-1}(R_2)$  to a coordinate plane  $\mathbf{R}^J$ , and let  $U \in O(p)$  be the matrix for which  $T = T_U$ . Then  $UR_2U^{-1} = I_\sigma$ , where  $\sigma = \sigma^J$ . For  $i = 1, 2$  let  $R'_i = UR_iU^{-1}$ . Since  $T$  is an orthogonal transformation, the (multi-)set of principal angles between  $E_{-1}(R'_1) = T(E_{-1}(R_1))$  and  $E_{-1}(R'_2) = T(E_{-1}(R_2))$  is identical to the (multi-)set of principal angles between  $E_{-1}(R_1)$  and  $E_{-1}(R_2)$ . But  $R'_1 I_\sigma = R'_1 R'_2 = UR_1 R_2 U^{-1}$ , so  $R(\theta_1, \dots, \theta_{\lceil p/2 \rceil})$  is a normal form of  $R'_1 I_\sigma$  as well as of  $R_1 R_2$ . The result now follows from Corollary 7.12(i) and equation (7.36) (the latter being needed only for the final statement of the result). ■

**Corollary 7.14** *The map  $\Phi = \Phi_{m,p} : (\text{Gr}_m(\mathbf{R}^p), d_{Gr}) \rightarrow (\text{Inv}_m(p), d_{SO(p)})$  (see (7.12)) is an isometry, up to a constant factor of 2:*

$$d_{SO(p)}(\Phi(W), \Phi(V)) = 2d_{Gr}(W, V) \quad (7.48)$$

for all  $W, V \in \text{Gr}_m(\mathbf{R}^p)$ .

**Proof:** Since  $d_{SO(p)}(RI_{\sigma}, I) = d_{SO(p)}(R, I_{\sigma}^{-1}) = d_{SO(p)}(R, I_{\sigma})$ , conclusion (ii) of Corollary 7.12 can be written equivalently as:

$$d_{SO(p)}(\Phi(W), \Phi(\mathbf{R}^J)) = 2d_{Gr}(W, \mathbf{R}^J). \quad (7.49)$$

Fix any  $J \in \mathcal{J}_{m,p}$ . Letting “ $\cdot$ ” denote the natural left-action of  $SO(p)$  on  $\text{Gr}_m(\mathbf{R}^p)$  ( $U \cdot W = T_U(W)$ , in the notation of the proof of Corollary 7.13), observe that for all  $U \in SO(p)$  and  $W \in \text{Gr}_m(\mathbf{R}^p)$ , we have  $\Phi(U \cdot W) = U\Phi(W)U^{-1}$  (simply another way of writing (7.47).) Clearly  $d_{Gr}$  is invariant under this action, and  $d_{SO(p)}$  is both left- and right-invariant, so (7.49) implies that

$$d_{SO(p)}(\Phi(U \cdot W), \Phi(U \cdot \mathbf{R}^J)) = 2d_{Gr}(U \cdot W, U \cdot \mathbf{R}^J).$$

Now let  $W, V \in \text{Gr}_m(\mathbf{R}^p)$ . Since the action of  $SO(p)$  on  $\text{Gr}_m(\mathbf{R}^p)$  is transitive, there exists  $U \in SO(p)$  such that  $U \cdot \mathbf{R}^J = V$ . Using any such  $U$ , we then have

$$\begin{aligned} d_{SO(p)}(\Phi(W), \Phi(V)) &= d_{SO(p)}(\Phi(U \cdot U^{-1} \cdot W), \Phi(U \cdot \mathbf{R}^J)) \\ &= 2d_{Gr}(U \cdot U^{-1} \cdot W, U \cdot \mathbf{R}^J) \\ &= 2d_{Gr}(W, V). \end{aligned}$$

■

**Remark 7.15** Of course, Corollary 7.49 can be deduced from computations with the principal fibration

$$\pi : SO(p) \rightarrow SO(p)/S(O(m) \times O(p-m)) \cong \text{Gr}_m(\mathbf{R}^p);$$

the standard Riemannian metric on  $\text{Gr}_m(\mathbf{R}^p)$  (for which  $d_{Gr}$  is the geodesic-distance function) is defined so as to make  $\pi$  a Riemannian submersion up to a normalization constant. The proof of Corollary 7.14 is independent of this Riemannian proof in the sense that it establishes equality between the left-hand side of (7.49) and the right-hand side *as defined by equation (7.15)*. Without the *a priori* knowledge that  $d_{Gr}$  is a geodesic-distance function, it is not obvious that  $d_{Gr}$  satisfies the triangle inequality, hence whether  $d_{Gr}$  is a metric. Thus Corollary 7.14 actually provides an independent proof that  $d_{Gr}$  is a metric on  $\text{Gr}_m(\mathbf{R}^p)$ . The only use of Riemannian geometry in this proof is through the knowledge that  $d_{SO(p)}$  is, in fact, a metric (because it is a geodesic-distance function).

**Proof of Proposition 7.7.** Let “Statement 1” and “Statement 2” be the statements listed as 1 and 2 in the Proposition. As noted in the proof of Corollary 7.14,  $d_{SO(p)}(RI_{\sigma}, I) = d_{SO(p)}(R, I_{\sigma})$ , so the inequality  $d_{SO(p)}(RI_{\sigma}, I) < d_{SO(p)}(R, I)$  can be rewritten as

$$d_{SO(p)}(R, I_{\sigma})^2 < \frac{m\pi^2}{2}.$$

Assume first that Statement 1 is true. Let  $W \in \text{Gr}_m(\mathbf{R}^p)$ . Then  $\Phi_{m,p}(W)$  is an involution of level  $m$ , so there exists  $\sigma \in \mathcal{I}_p^+$  of level  $m$  such that  $d_{SO(p)}(\Phi_{m,p}(W), I_\sigma)^2 < \frac{m\pi^2}{2}$ . Select such a  $\sigma$  and let  $J = J^\sigma$ . Then  $I_\sigma = \Phi_{m,p}(\mathbf{R}^J)$ , so

$$\begin{aligned} d_{Gr}(W, \mathbf{R}^J)^2 &= \frac{1}{4} d_{SO(p)}(\Phi_{m,p}(W), \Phi_{m,p}(\mathbf{R}^J))^2 = \frac{1}{4} d_{SO(p)}(\Phi_{m,p}(W), I_\sigma)^2 \\ &< \frac{m\pi^2}{8}. \end{aligned}$$

Hence Statement 2 is true.

Conversely, assume that Statement 2 is true. Let  $R \in \text{Inv}_m(p)$ . Then there exists  $J \in \mathcal{J}_{m,p}$  such that  $d_{Gr}(\Phi_{m,p}^{-1}(R), \mathbf{R}^J)^2 < \frac{m\pi^2}{8}$ . Select such a  $J$  and let  $\sigma = \sigma^J$ . Then  $I_\sigma = \Phi_{m,p}(\mathbf{R}^J)$ , so

$$d_{SO(p)}(R, I_\sigma)^2 = d_{SO(p)}(R, \Phi_{m,p}(\mathbf{R}^J))^2 = 4d_{Gr}(\Phi_{m,p}^{-1}(R), \mathbf{R}^J)^2 < \frac{m\pi^2}{2}.$$

Hence Statement 1 is true. ■

We are now ready to attack the question of sign-change reducibility: given  $R \in \text{Inv}(p)$ , can we find  $\sigma \in \mathcal{I}_p^+$  such that  $d_{SO(p)}(RI_\sigma, I) < d_{SO(p)}(R, I)$ ? Equations (7.11) and (7.33) tell us that this inequality is satisfied if and only if

$$(l_+ + l_-)\pi^2 + 2 \sum_{j \in J_*} \tilde{\theta}_j^2 < \text{level}(R)\pi^2, \quad (7.50)$$

where  $l_\pm = l_\pm(R, \sigma)$  are as in Lemma 7.10(vii). Since  $\pi$  is the largest possible value for a normal-form angle in (7.1), it is reasonable to try to look for a  $\sigma$  such that  $l_+$  and  $l_-$  are as small as possible. However, to achieve (7.50), we have to make sure that we do not make  $\sum_{j \in J_*} \tilde{\theta}_j^2$  too large while we are making  $l_\pm$  small. We next prove a lemma that, via its subsequent corollary, will help us show that for  $\text{level}(R) = m \geq \frac{p}{2}$ , we can choose  $J \in \mathcal{J}_{m,p}$  to make  $d_{SO(p)}(RI_{\sigma^J}, I)$  as small as is needed to prove Proposition 7.5.

**Lemma 7.16** *For  $1 \leq m \leq p$ ,*

$$\sum_{J \in \mathcal{J}_{m,p}} \mathbf{E}_J \mathbf{E}_J^T = \binom{p-1}{m-1} I_{p \times p}. \quad (7.51)$$

**Proof:** For  $J = (i_1, \dots, i_m) \in \mathcal{J}_{m,p}$ , we have

$$\mathbf{E}_J \mathbf{E}_J^T = \sum_{i \in J} \mathbf{e}_i \mathbf{e}_i^T. \quad (7.52)$$

Hence when  $m = 1$  and when  $m = p$ , the left-hand side of (7.51) reduces to  $I_{p \times p}$ , which is also true of the right-hand side.

We proceed by induction on  $p$ . For each  $p \geq 1$ , consider the statement

$$S(p) : \text{Equation (7.51) is true for all } m \text{ satisfying } 1 \leq m \leq p. \quad (7.53)$$

We have already established that (7.51) holds for  $m = 1 = p$ , hence that statement  $S(1)$  is true. Now suppose that  $S(p)$  is true for some given  $p$ . To consider  $S(p+1)$ , let  $\{\mathbf{e}_i\}_{i=1}^p, \{\mathbf{e}'_i\}_{i=1}^{p+1}$  denote the standard bases of  $\mathbf{R}^p, \mathbf{R}^{p+1}$  respectively. For  $K = \{i_1, \dots, i_m\} \in \mathcal{J}_{p+1,m}$  with  $i_1 < i_2 < \dots < i_m$  we write  $E'_K$  for the  $(p+1) \times m$  matrix whose  $j^{\text{th}}$  column is  $\mathbf{e}'_{i_j}$ ,  $1 \leq j \leq m$ . Note that

$$\begin{aligned} \mathbf{e}'_i &= \begin{bmatrix} \mathbf{e}_i \\ 0 \end{bmatrix} \quad \text{for } 1 \leq i \leq p, \\ E'_J(E'_J)^T &= \begin{bmatrix} E_J(E_J)^T & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} \quad \text{for } J \in \mathcal{J}_{m,p}, \\ \text{and} \quad \mathbf{e}'_{p+1}(\mathbf{e}'_{p+1})^T &= \begin{bmatrix} 0_{p \times p} & 0_{p \times 1} \\ 0_{1 \times p} & 1 \end{bmatrix}. \end{aligned}$$

Hence for  $1 \leq m \leq p$ ,

$$\begin{aligned} & \sum_{K \in \mathcal{J}_{m,p+1}} E'_K(E'_K)^T \\ &= \sum_{\{K \in \mathcal{J}_{m,p+1} : p+1 \in K\}} E'_K(E'_K)^T + \sum_{\{K \in \mathcal{J}_{m,p+1} : p+1 \notin K\}} E'_K(E'_K)^T \\ &= \sum_{\{K \in \mathcal{J}_{m,p+1} : K = J \cup \{p+1\} \text{ for some } J \in \mathcal{J}_{m-1,p}\}} E'_K(E'_K)^T + \sum_{K \in \mathcal{J}_{m,p}} E'_K(E'_K)^T \\ &= \sum_{J \in \mathcal{J}_{m-1,p}} (E'_J(E'_J)^T + \mathbf{e}'_{p+1}(\mathbf{e}'_{p+1})^T) + \sum_{J \in \mathcal{J}_{m,p}} \begin{bmatrix} E_J(E_J)^T & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} \\ &= \sum_{J \in \mathcal{J}_{m-1,p}} \left( \begin{bmatrix} E_J E_J^T & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} \right) + |\mathcal{J}_{m-1,p}| \mathbf{e}'_{p+1}(\mathbf{e}'_{p+1})^T \\ &\quad + \sum_{J \in \mathcal{J}_{m,p}} \begin{bmatrix} E_J(E_J)^T & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} \\ &= \begin{bmatrix} \sum_{J \in \mathcal{J}_{m-1,p}} E_J E_J^T + \sum_{J \in \mathcal{J}_{m,p}} E_J E_J^T & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} \\ &\quad + |\mathcal{J}_{m-1,p}| \mathbf{e}'_{p+1}(\mathbf{e}'_{p+1})^T \\ &= \begin{bmatrix} \left\{ \binom{p-1}{m-2} + \binom{p-1}{m-1} \right\} I_{p \times p} & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} + \binom{p}{m-1} \mathbf{e}'_{p+1}(\mathbf{e}'_{p+1})^T \\ &= \binom{p}{m-1} \left\{ \begin{bmatrix} I_{p \times p} & 0_{p \times 1} \\ 0_{1 \times p} & 0 \end{bmatrix} + \mathbf{e}'_{p+1}(\mathbf{e}'_{p+1})^T \right\} \\ &= \binom{p}{m-1} I_{(p+1) \times (p+1)} \end{aligned}$$

Hence (7.16) holds with  $p$  replaced by  $p + 1$ , as long as  $1 \leq m \leq p$ . But we have already established that (7.16) holds whenever  $m = p$ ; hence if  $p$  is replaced by  $p + 1$ , the equality holds for  $m = p + 1$ . Thus (7.16) holds for all  $m$  with  $1 \leq m \leq p + 1$ ; i.e. statement  $S(p + 1)$  is true. By induction,  $S(p)$  is true for all  $p$ , which is exactly what the Lemma asserts. ■

**Corollary 7.17** *Let  $m \in \{1, 2, \dots, p\}$  and let  $W \in \text{Gr}_m(\mathbf{R}^p)$ . There exists  $J \in \mathcal{J}_{m,p}$  such that*

$$\sum_{i=1}^m \sin^2 \phi_{J,i} \leq m \left(1 - \frac{m}{p}\right). \quad (7.54)$$

Furthermore, the inequality in (7.54) is strict for some  $J \in \mathcal{J}_{m,p}$  unless equality holds in (7.54) for all  $J \in \mathcal{J}_{m,p}$ .

**Proof:** Let  $\widetilde{W}$  be any  $p \times m$  matrix whose columns are an orthonormal basis of  $W$ . Using Lemma 7.16,

$$\begin{aligned} \sum_{J \in \mathcal{J}_{m,p}} \text{tr}(\widetilde{W}^T \mathbf{E}_J \mathbf{E}_J^T \widetilde{W}) &= \text{tr} \left( \widetilde{W}^T \left( \sum_{J \in \mathcal{J}_{m,p}} \mathbf{E}_J \mathbf{E}_J^T \right) \widetilde{W} \right) \\ &= \text{tr} \left( \widetilde{W}^T \binom{p-1}{m-1} I_{p \times p} \widetilde{W} \right) \\ &= m \binom{p-1}{m-1} \end{aligned}$$

since  $\widetilde{W}^T \widetilde{W} = I_{m \times m}$ .

Since  $|\mathcal{J}_{m,p}| = \binom{p}{m}$ , the average of  $\text{tr}(\widetilde{W}^T \mathbf{E}_J \mathbf{E}_J^T \widetilde{W})$  over all  $J \in \mathcal{J}_{m,p}$  is  $m \binom{p-1}{m-1} / \binom{p}{m} = m^2/p$ . Hence  $\text{tr}(\widetilde{W}^T \mathbf{E}_J \mathbf{E}_J^T \widetilde{W}) \geq m^2/p$  for at least one  $J \in \mathcal{J}_{m,p}$ , and the inequality is strict for some  $J$  unless it is an equality for all  $J$ . But for any  $Z \in \text{Gr}_m(\mathbf{R}^p)$ , the principal angles  $\phi_1, \dots, \phi_m$  between  $W$  and  $Z$  are the numbers in  $[0, \frac{\pi}{2}]$  for which  $\cos \phi_1, \dots, \cos \phi_m$  are the singular values of the  $m \times m$  matrix  $\widetilde{W}^T \widetilde{Z}$ , where  $\widetilde{Z}$  is any  $p \times m$  matrix whose columns are an orthonormal basis of  $Z$ . Since for any  $J \in \mathcal{J}_{m,p}$  the columns of  $\mathbf{E}_J$  are an orthonormal basis of  $\mathbf{R}^J$ , it follows that  $\sum_{i=1}^m \cos^2 \phi_{J,i} = \text{tr}(\widetilde{W}^T \mathbf{E}_J (\widetilde{W}^T \mathbf{E}_J)^T) = \text{tr}(\widetilde{W}^T \mathbf{E}_J \mathbf{E}_J^T \widetilde{W})$ . Thus, for some  $J$ ,  $\sum_{i=1}^m \cos^2 \phi_{J,i} \geq \frac{m^2}{p}$ , and the inequality is strict for some  $J$  unless it is an equality for all  $J$ . But for any given  $J$ ,

$$\sum_{i=1}^m \cos^2 \phi_{J,i} \geq \frac{m^2}{p} \iff \sum_{i=1}^m \sin^2 \phi_{J,i} = m - \sum_{i=1}^m \cos^2 \phi_{J,i} \leq m - \frac{m^2}{p} = m \left(1 - \frac{m}{p}\right), \quad (7.55)$$

and the first inequality in (7.55) is strict if and only if the second is strict. Thus (7.54) holds for some  $J$ , and the inequality in (7.54) is strict for some  $J$  unless it is an equality for all  $J$ . ■



**Proof of Proposition 7.5.**

If  $m = p$  then  $p$  is even,  $R = -I$ , and for  $\sigma = (-1, -1, \dots, -1)$  we have  $I_\sigma = -I$  and  $d_{SO(p)}(RI_\sigma, I) = 0 < d_{SO(p)}(R, I)$ . Henceforth we assume  $m < p$ .

Let  $W = E_{-1}(R)$  and let  $m = \dim(W)$ . Note that

$$d_{SO(p)}(R, I)^2 = \frac{m}{2}\pi^2. \quad (7.56)$$

Let  $J \in \mathcal{J}_{m,p}$  be such that  $\sum_{i=1}^m \sin^2 \phi_{J,i} = \min_{K \in \mathcal{J}_{m,p}} \{\sum_{i=1}^m \sin^2 \phi_{K,i}\}$ . By Corollary 7.17, inequality (7.54) holds, and the inequality is strict unless

$$\sum_{i=1}^m \sin^2 \phi_{K,i} = m(1 - \frac{m}{p}) \quad (7.57)$$

for all  $K \in \mathcal{J}_{m,p}$ . Let  $\sigma = \sigma^J$ . By Corollary 7.12,

$$d_{SO(p)}(RI_\sigma)^2 = 4d_{Gr}(W, \mathbf{R}^J)^2 = 4 \sum_{i=1}^m (\phi_{J,i})^2 \quad (7.58)$$

where  $\phi_{J,i} = \phi_{J,i}(W)$ .

The function  $f : x \mapsto \frac{\sin x}{x}$  is strictly decreasing on the interval  $(0, \frac{\pi}{2}]$ . Hence for all  $x \in (0, \frac{\pi}{2}]$  we have  $\frac{\sin x}{x} \geq f(\frac{\pi}{2}) = \frac{2}{\pi}$ , with equality only if  $x = \frac{\pi}{2}$ ; thus for  $x \in [0, \frac{\pi}{2}]$  we have  $x \leq \frac{\pi}{2} \sin x$ , with equality only if  $x = 0$  or  $x = \frac{\pi}{2}$ . Hence

$$d_{SO(p)}(RI_\sigma)^2 = 4 \sum_{i=1}^m (\phi_{J,i})^2 \leq \pi^2 \sum_{i=1}^m \sin^2 \phi_{J,i} \quad (7.59)$$

$$\leq m(1 - \frac{m}{p})\pi^2 \quad (7.60)$$

$$\leq \frac{m}{2}\pi^2 \quad (\text{since } \frac{m}{p} \geq \frac{1}{2}) \quad (7.61)$$

$$= d_{SO(p)}(R, I)^2.$$

Hence  $d_{SO(p)}(RI_\sigma) \leq d_{SO(p)}(R, I)$ , and this inequality is strict if any of the inequalities (7.59), (7.60), (7.61) is strict. Inequality (7.59) is strict if  $0 < \phi_{J,i} < \frac{\pi}{2}$  for some  $i$ , and, by our choice of  $J$ , (7.60) is strict unless equality holds in (7.57) for all  $K \in \mathcal{J}_{m,p}$ .

We claim that at least one of the inequalities (7.59), (7.60) is strict. Assume this is not so. Then, since equality holds in (7.59) with  $J$  replaced by any  $K \in \mathcal{J}_{m,p}$ , it follows that for all  $K \in \mathcal{J}_{m,p}$  and  $i \in \{1, \dots, m\}$  the angle  $\phi_{K,i}$  is either 0 or  $\pi/2$ , and that  $\sum_{i=1}^m \sin^2 \phi_{K,i} = m(1 - \frac{m}{p})$  for all  $K$ . But for any  $V \in \text{Gr}_m(\mathbf{R}^p)$ , there always exists  $K \in \mathcal{J}_{m,p}$  for which none of the principal angles  $\phi_{K,i}(V, \mathbf{R}^K)$  is  $\pi/2$ . Choosing such  $K$  for our  $m$ -plane  $W$ , all of the principal angles  $\phi_{K,i}$  must therefore be 0 (since they are all either 0 or  $\pi/2$ ). But then  $\sum_{i=1}^m \sin^2 \phi_{K,i} = 0 < m(1 - \frac{m}{p})$ , a contradiction.

Thus at least one of the inequalities (7.59), (7.60) is strict, so  $d_{SO(p)}(RI_\sigma) < d_{SO(p)}(R, I)$ . ■

As noted earlier, Proposition 7.5 proves Proposition 4.13(a). To prove Proposition 4.13(b), we start with a weakened version of Conjecture 7.6:

**Proposition 7.18** *Let  $m \geq 2$  be even, let  $R \in SO(p)$  be an involution of level  $m$ , and let  $\sigma \in \mathcal{I}_p^+$ . If  $d_{SO(p)}(RI\sigma, I) < d_{SO(p)}(R, I)$ , then  $\text{level}(\sigma) < 2m$ . (Hence if  $R$  is sign-change reducible, then it is reducible by a sign-change of level less than  $2m$ ).*

**Proof:** Let  $m_\sigma = \text{level}(\sigma)$ . Define  $l_\pm$  as in Lemma 7.10. From (7.33),

$$\frac{1}{2}(l_+ + l_-)\pi^2 \leq d_{SO(p)}(RI\sigma, I)^2 < d_{SO(p)}(R, I)^2 = \frac{1}{2}m_R\pi^2,$$

so

$$l_+ + l_- < m_R. \quad (7.62)$$

But by (7.19) we have  $l_- = l_+ + m_\sigma - m_R$ , so substituting into (7.62), we have  $2l_+ + m_\sigma - m_R < m_R$ ; equivalently,

$$2l_+ < 2m_R - m_\sigma.$$

Since  $l_+ \geq 0$ , we must have  $m_\sigma < 2m_R$ . ■

**Corollary 7.19** *Conjecture 7.6 is true for  $m = 2$ .*

**Proof:** The only positive even integer less than  $2 \times 2$  is 2. ■

The combination of Corollary 7.19 and Proposition 7.7 is what will guide our proof of Proposition 4.13(b). To prove Proposition 4.13(b), it suffices to prove that for  $p \geq 11$ , the answer to Question 7.4 is “no”—i.e. that there exist involutions in  $SO(p)$  that are not sign-change reducible. Hence it suffices to prove that there exist such involutions of level 2. By Corollary 7.19, it therefore suffices to establish (for  $p \geq 11$ ) the existence of involutions that are not sign-change reducible by a sign-change of level 2; thus it suffices to show that Statement 2 of Proposition 7.7 is false when  $p \geq 11$  and  $m = 2$ . For this, we need only produce planes in  $\mathbf{R}^p$  for which we can show that (7.13) is false for all  $J \in \mathcal{J}_{2,p}$ . Towards this end, we examine two (families) of examples in which  $m = 2$  and  $p \geq 4$ .

**Example 7.20** Let  $p = 2k$  or  $2k + 1$ , where  $k \geq 2$ . Define vectors  $\hat{v}, \hat{w} \in \mathbf{R}^p$  by

$$\hat{v} = \frac{1}{\sqrt{k}} \sum_{i=1}^k \mathbf{e}_i, \quad \hat{w} = \frac{1}{\sqrt{k}} \sum_{i=k+1}^{2k} \mathbf{e}_i.$$

The set  $\{\hat{v}, \hat{w}\}$  is orthonormal. Let  $W_p = \text{span}\{\hat{v}, \hat{w}\}$ , a 2-plane in  $\mathbf{R}^p$ . We will compute the principal angles between  $W_p$  and  $\mathbf{R}^J$  for all  $J \in \mathcal{J}_{2,p}$ . Write  $J = \{i, j\}$ , where  $1 \leq i < j \leq p$ . Let  $\widetilde{W}$  be the  $p \times 2$  matrix whose first column is  $\hat{v}$  and whose second column is  $\hat{w}$ . Since the columns of  $\widetilde{W}$  are an orthonormal basis of  $W_p$ , the principal angles between  $W_p$  and  $\mathbf{R}^J$  are the arc-cosines of the singular values of  $\widetilde{W}^T \mathbf{E}_J$ .

First suppose that  $p$  is even. We divide the elements  $\{i, j\} \in \mathcal{J}_{2,p}$  into two cases: Case I =  $\{\{i, j\} : i < j \leq k \text{ or } k < i < j\}$ ; Case II =  $\{\{i, j\} : i \leq k < j\}$ . The principal values of the  $2 \times 2$  matrix  $\widetilde{W}^T \mathbf{E}_J$  are easily computed to be 0 and  $\frac{4}{p}$  in Case I, and  $\frac{2}{p}$  (with multiplicity 2) in Case II. Hence the principal angles are

$$\begin{aligned} \phi_{J,1} &= \frac{\pi}{2}, \quad \phi_{J,2} = \cos^{-1} \sqrt{4/p} \text{ in Case I,} \\ \phi_{J,1} &= \phi_{J,2} = \cos^{-1} \sqrt{2/p} \text{ in Case II,} \end{aligned}$$

so

$$\min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W_p, \mathbf{R}^J)^2\} = \min \left\{ \left(\frac{\pi}{2}\right)^2 + \left(\cos^{-1} \sqrt{4/p}\right)^2, 2 \left(\cos^{-1} \sqrt{2/p}\right)^2 \right\}. \quad (7.63)$$

We will return to (7.63) shortly, but first let us do the analogous computation for  $p$  odd. For  $p = 2k + 1$ , we divide the computation into three cases: Case I =  $\{\{i, j\} : i < j \leq k \text{ or } k < i < j \leq 2k\}$ ; Case II =  $\{\{i, j\} : i \leq k < j \leq 2k\}$ ; and Case III =  $\{\{i, j\} : i \leq 2k, j = 2k + 1\}$ . The principal values of the matrix  $\widetilde{W}^T \mathbf{E}_J$  are 0 and  $\frac{2}{p} + \frac{2}{p-1}$  in Case I,  $\frac{2}{p}$  and  $\frac{2}{p-1}$  in Case II, and  $\frac{2}{p-1}$  in Case III. Hence the principal angles are

$$\begin{aligned} \phi_{J,1} &= \frac{\pi}{2}, \quad \phi_{J,2} = \cos^{-1} \sqrt{4/(p-1)} \text{ in Case I,} \\ \phi_{J,1} &= \phi_{J,2} = \cos^{-1} \sqrt{2/(p-1)} \text{ in Case II,} \\ \phi_{J,1} &= \frac{\pi}{2}, \quad \phi_{J,2} = \cos^{-1} \sqrt{2/(p-1)} \text{ in Case III.} \end{aligned}$$

Clearly  $\phi_{J,1}^2 + \phi_{J,2}^2$  is larger in Case III than in Case II, so

$$\min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W_p, \mathbf{R}^J)^2\} = \min \left\{ \left(\frac{\pi}{2}\right)^2 + \left(\cos^{-1} \sqrt{\frac{4}{p-1}}\right)^2, 2 \left(\cos^{-1} \sqrt{\frac{2}{p-1}}\right)^2 \right\}. \quad (7.64)$$

It follows from (7.63) and (7.64) that

$$\begin{aligned} \lim_{p \rightarrow \infty} \min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W_p, \mathbf{R}^J)^2\} &= 2 \left(\frac{\pi}{2}\right)^2 = \frac{\pi^2}{2} \\ &\not\leq \frac{\pi^2}{4} = \frac{m\pi^2}{8} \end{aligned} \quad (7.65)$$

since  $m = 2$  in Example 7.20. Hence for large enough  $p$ , Statement 2 in Proposition 7.7 is false, and therefore so is Statement 1. This already shows that for all  $p$  sufficiently large, there exist geodesically antipodal pairs  $(U, V)$  in  $SO(p) \times SO(p)$  that are not sign-change reducible. However, to get the quantitative statement in Proposition 4.13(b), we have to continue working.

It can be shown<sup>4</sup> that for  $0 < x \leq 1$ ,

<sup>4</sup>The authors did not find this exercise in Calculus 1 entirely trivial, but are nonetheless leaving it to the reader.

$$(\pi/2)^2 + (\cos^{-1} x)^2 > 2(\cos^{-1} \frac{x}{\sqrt{2}})^2, \quad (7.66)$$

hence that in (7.63) in (7.64), the second of the two expressions being compared is the smaller. Thus

$$\min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W_p, \mathbf{R}^J)\} = \sqrt{2} \cos^{-1}(c_p), \quad \text{where } c_p = \begin{cases} \sqrt{2/p}, & p \text{ even}, \\ \sqrt{2/(p-1)}, & p \text{ odd}. \end{cases} \quad (7.67)$$

Since  $m = 2$  in Example 7.20,  $\sqrt{m\pi^2/8} = \frac{\pi}{2}$ , so equation (7.67) shows that (7.13) (with  $W = W_p$ ) is false for all  $J \in \mathcal{J}_{2,p}$  if  $\sqrt{2} \cos^{-1}(c_p) \geq \frac{\pi}{2}$ ; equivalently, if  $c_p \leq \cos \frac{\pi}{2\sqrt{2}} \approx 0.4440$ . This translates to  $2\lfloor \frac{p}{2} \rfloor \geq 2 \sec^2 \frac{\pi}{2\sqrt{2}} \approx 10.14$ . Hence the answer to Question 7.4 is definitely “no” for all  $p \geq 12$ . To complete the proof of Proposition 4.13(b), it remains only to show that this “12” can be reduced to “11”. We will accomplish this with the next example.

**Example 7.21** Let  $p = 2k + 1$ , where  $k \geq 2$ . Define vectors  $v, w, \hat{v}, \hat{w} \in \mathbf{R}^p$  by

$$\begin{aligned} v &= \sum_{i=1}^p \mathbf{e}_i, & w &= \sum_{i=1}^k \mathbf{e}_i - \sum_{i=k+1}^{2k} \mathbf{e}_i \\ \hat{v} &= \frac{v}{\|v\|} = \frac{1}{\sqrt{p}} v, & \hat{w} &= \frac{w}{\|w\|} = \frac{w}{\sqrt{p-1}}. \end{aligned}$$

As in the previous example,  $\{\hat{v}, \hat{w}\}$  is an orthonormal basis of a plane  $W'_p$ . Just as in Example 7.20, we can compute the principal angles between  $W'_p$  and  $\mathbf{R}^J$  for all  $J \in \mathcal{J}_{2,p}$ . We define Cases I and II and III just as in the odd- $p$  case of the previous example. The principal values of the relevant  $2 \times 2$  matrices are 0 and  $\frac{2}{p} + 2/(p-1)$  in Case I,  $\frac{2}{p}$  and  $\frac{2}{p-1}$  in Case II, and

$$\lambda_{\pm}(p) := \frac{1}{p} + \frac{1}{2(p-1)} \pm \sqrt{\frac{1}{p^2} + \frac{1}{4(p-1)^2}}$$

in Case III. Hence

$$\begin{aligned} \min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W'_p, \mathbf{R}^J)^2\} &= \min \left\{ \left( \frac{\pi}{2} \right)^2 + \left( \cos^{-1} \sqrt{\frac{2}{p} + \frac{2}{p-1}} \right)^2, \right. \\ &\quad \left( \cos^{-1} \sqrt{2/p} \right)^2 + \left( \cos^{-1} \sqrt{2/(p-1)} \right)^2, \\ &\quad \left. \left( \cos^{-1}(\sqrt{\lambda_+(p)}) \right)^2 + \left( \cos^{-1}(\sqrt{\lambda_-(p)}) \right)^2 \right\} \end{aligned} \quad (7.68)$$

Numerically, we find that for  $p = 11$ , the middle line of (7.68) is the smallest

of the three lines, so

$$\begin{aligned} \min_{J \in \mathcal{J}_{2,11}} \{d_{Gr}(W'_{11}, \mathbf{R}^J)^2\} &= \left(\cos^{-1} \sqrt{2/11}\right)^2 + \left(\cos^{-1} \sqrt{2/10}\right)^2 \\ &\approx 1.0146 \frac{\pi^2}{4}. \end{aligned} \quad (7.69)$$

Since this number is larger than  $\frac{\pi^2}{4}$ , the answer to Question 7.4 is “no” for  $p = 11$ . This completes the proof of Proposition 4.13(b). ■

**Remarks 7.22** 1. We considered Example 7.21 only for odd  $p$  because for even  $p$ , the principal angles  $\phi_{J,i}(W'_p)$  turn out to be the same as for  $\phi_{J,i}(W_p)$  in Example 7.20. In Example 7.21, we can also compute numerically that for  $p = 5, 7$ , and 9, we have  $\min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W'_p, \mathbf{R}^J)^2\} < \frac{\pi^2}{4}$ . However, we cannot conclude that the answer to Question 7.4 is “yes” for  $p \leq 10$ , since we have not proven that this example represents the worst case, i.e. that  $\min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W'_p, \mathbf{R}^J)\} \geq \min_{J \in \mathcal{J}_{2,p}} \{d_{Gr}(W, \mathbf{R}^J)\}$  for all  $W \in \text{Gr}_m(\mathbf{R}^p)$ . Thus Question 7.4 remains open for  $5 \leq p \leq 10$ . However, based on computations, it seems likely to the authors that the largest  $p$  for which the answer to Question 7.4 is likely to be closer to 10 than to 4.

2. The number  $\frac{\pi^2}{2}$  in (7.65) is exactly the squared diameter of  $\text{Gr}_2(\mathbf{R}^p)$  for all  $p \geq 4$ . Thus, (7.65) shows that as  $p \rightarrow \infty$ , the distance between  $W_p$  and the *closest* coordinate plane(s)  $\mathbf{R}^J$  is approaching the *largest* possible distance between two points in  $\text{Gr}_2(\mathbf{R}^p)$ .

#### 7.4. Proof of Proposition 4.15

**Lemma 7.23** Let  $c > 0$ . There exist  $D, \Lambda \in \mathcal{D}_{\text{top}} := \mathcal{D}_{\text{J}_{\text{top}}}$  such that  $\|\log(D^{-1}(\pi \cdot \Lambda))\|^2 > \|\log(D^{-1}\Lambda)\|^2 + c$  for all non-identity  $\pi \in S_p$ .

**Proof:** Let  $c_1 = \sqrt{c/(3p)}$  and let  $\{a_i\}_{i=1}^p$  be a sequence of numbers satisfying  $a_{i+1} - a_i > (2\sqrt{p} + 1)c_1$  for  $1 \leq i \leq p-1$ . Then  $|c + a_j - a_i| > 2\sqrt{p}c$  for all  $i \neq j$ . Let  $D = \text{diag}(e^{a_1}, \dots, e^{a_p})$  and let  $\Lambda = e^{c_1} D$ . Then  $D, \Lambda \in \mathcal{D}_{\text{top}}$  and  $\|\log(D^{-1}\Lambda)\|^2 = \|c_1 I\|^2 = pc_1^2$ .

Let  $\pi \in S_p, \pi \neq \text{id}$ , and let  $i$  be such that  $\pi^{-1}(i) \neq i$ . Then

$$\|\log(D^{-1}(\pi \cdot \Lambda))\|^2 \geq |c_1 + a_{\pi^{-1}(i)} - a_i|^2 > (2\sqrt{p}c_1)^2 = \|\log(D^{-1}\Lambda)\|^2 + c.$$

■

**Proof of Proposition 4.15.** Let  $D, \Lambda \in \mathcal{D}_{\text{top}}$  such that

$$\|\log(D^{-1}(\pi \cdot \Lambda))\|^2 > \|\log(D^{-1}\Lambda)\|^2 + k \text{diam}(SO(p))^2 \quad (7.70)$$

for all non-identity  $\pi \in S_p$ ; such  $D, \Lambda$  exist by Lemma 7.23. Let  $X = F(U, D), Y = F(V, \Lambda)$ . The subgroups  $G_D^0, G_\Lambda^0$  of  $SO(p)$  are trivial (i.e., contain only the identity element), as are the subgroups  $\Gamma_{J_D}^0$  and  $\Gamma_{J_\Lambda}^0$  of  $\tilde{S}_p^+$ . Hence in Proposition 4.9 we have  $Z = \tilde{S}_p^+$  and

$$\begin{aligned} d_{S\mathcal{R}}(X, Y)^2 &= \min_{g \in \tilde{S}_p^+} \left\{ k d_{SO(p)}(U, VP_g^{-1})^2 + \|\log(D^{-1}(\pi_g \cdot \Lambda))\|^2 \right\} \\ &= \min_{\pi \in \tilde{S}_p^+} \left\{ k \min_{g \in \tilde{S}_p^+, \pi_g = \pi} \left\{ d_{SO(p)}(U, VP_g^{-1})^2 + \|\log(D^{-1}(\pi \cdot \Lambda))\|^2 \right\} \right\}. \end{aligned}$$

For all non-identity  $\pi \in S_p$  and all  $g_1, g_2 \in \tilde{S}_p^+$  with  $\pi_{g_1} = \text{id.}$  and  $\pi_{g_2} = \pi$ , using (7.70) we then have

$$\begin{aligned} d_M((U, D), (VP_{g_1}^{-1}, \pi_{g_1} \cdot \Lambda))^2 &= k d_{SO(p)}(U, VP_{g_1}^{-1})^2 + \|\log(D^{-1}\Lambda)\|^2 \\ &\leq k \text{diam}(SO(p))^2 + \|\log(D^{-1}\Lambda)\|^2 \\ &< \|\log(D^{-1}(\pi \cdot \Lambda))\|^2 \\ &\leq d_M((U, D), (VP_{g_2}^{-1}, \pi_{g_2} \cdot \Lambda))^2. \end{aligned}$$

Hence the identity permutaton is the only element of  $S_p$  for which the expression inside the outer braces in (7.71) achieves the minimum over all  $\pi \in S_p$ . But  $\{g \in \tilde{S}_p^+ : \pi_g = \text{id.}\}$  is precisely the sign-change subgroup  $\mathcal{I}_p^+$ , and by hypothesis  $(U, V)$  is not sign-change reducible. Hence

$$\begin{aligned} d_{S\mathcal{R}}(X, Y)^2 &= \min_{\sigma \in \mathcal{I}_p^+} \left\{ k d_{SO(p)}(U, VI_\sigma)^2 + \|\log(D^{-1}\Lambda)\|^2 \right\} \\ &= k d_{SO(p)}(U, V)^2 + \|\log(D^{-1}\Lambda)\|^2 \\ &= d_M((U, D), (V, \Lambda))^2. \end{aligned}$$

Thus  $((U, D), (V, \Lambda))$  is a minimal pair. ■

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# Supplementary Material to Eigenvalue stratification and minimal smooth scaling-rotation curves in the space of symmetric positive-definite matrices<sup>\*</sup>

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## 1. Scaling–Rotation distance and MSSR curves in $\text{Sym}^+(2)$

The space  $\text{Sym}^+(2)$  has only two strata:  $\mathcal{S}_{\text{bot}} := \mathcal{S}_{[\text{j}_{\text{bot}}]} = \{\lambda I_2 : \lambda > 0\}$  and  $\mathcal{S}_{\text{top}} := \mathcal{S}_{[\text{j}_{\text{top}}]} = \text{Sym}^+(2) \setminus \mathcal{S}_{\text{bot}}$ . To characterize all unique and non-unique cases of minimal smooth scaling-rotation (MSSR) curves in  $\text{Sym}^+(2)$ , it suffices to consider two possibilities for the strata in which  $X, Y$  lie:

- (i)  $X, Y \in \mathcal{S}_{\text{top}}$ .
- (ii)  $X \in \mathcal{S}_{\text{bot}}$  ( $Y \in \mathcal{S}_{\text{top}} \cup \mathcal{S}_{\text{bot}} = \text{Sym}^+(2)$ ).

For any  $X, Y \in \text{Sym}^+(2)$ , with  $a \geq b$ ,  $c \geq d$  and  $0 \leq \theta < \pi$ , one can write

$$X = U \begin{pmatrix} e^a & 0 \\ 0 & e^b \end{pmatrix} U^T, \quad Y = U R_\theta \begin{pmatrix} e^c & 0 \\ 0 & e^d \end{pmatrix} R_\theta^T U^T \quad (1)$$

where  $U \in \text{SO}(2)$  and  $R_\theta = \exp(A_\theta)$ ,  $A_\theta = \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix}$ . Denote the apparent eigen-decompositions of  $X$  and  $Y$  appearing in (1) by  $(U, D)$  and  $(V, \Lambda)$ . Then the scaling–rotation curve  $\chi$  with parameters  $(U, D, A, L)$ ,  $A = \log(VU^T)$  and  $L = \exp(D^{-1}\Lambda)$  is

$$\chi(t) = (U R_{\theta t}) \exp \begin{pmatrix} (1-t)a + tc & 0 \\ 0 & (1-t)b + td \end{pmatrix} (U R_{\theta t})^T, \quad (2)$$

---

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satisfying  $\chi(0) = X$ ,  $\chi(1) = Y$ .

**Case (i).** ( $a > b$ ,  $c > d$ ) Let  $(V_i, \Lambda_i)$ ,  $i = 1, \dots, 4$  be the four eigen-decompositions of  $Y$ . Specifically, these four eigen-decompositions are

$$\begin{aligned} (V_1, \Lambda_1) &= (UR_\theta, \text{diag}(e^c, e^d)), \\ (V_2, \Lambda_2) &= (UR_{\theta+\pi}, \text{diag}(e^c, e^d)), \\ (V_3, \Lambda_3) &= (UR_{\theta+\pi/2}, \text{diag}(e^d, e^c)), \\ (V_4, \Lambda_4) &= (UR_{\theta-\pi/2}, \text{diag}(e^d, e^c)). \end{aligned}$$

Then  $d_{\mathcal{SR}}(X, Y) = \min_{i=1,2,3,4} d_i$ , where  $d_i = d((U, D), (V_i, \Lambda_i))$ . For  $0 \leq \theta \leq \pi/2$ ,

$$d_1^2 = k\theta^2 + (a-c)^2 + (b-d)^2 \leq d_2^2,$$

and equality holds if and only if  $\theta = \pi/2$ . On the other hand, if  $\pi/2 < \theta < \pi$ ,

$$d_2^2 = k(\pi - \theta)^2 + (a-c)^2 + (b-d)^2 < d_1^2,$$

For  $0 \leq \theta < \pi$ ,

$$d_3^2 = k(\theta - \pi/2)^2 + (a-d)^2 + (b-c)^2 \leq d_4^2,$$

and equality holds if and only if  $\theta = 0$ . Furthermore, we have

$$\begin{aligned} d_1^2 < d_3^2 &\iff \theta < \frac{\pi}{4} + \frac{2(a-b)(c-d)}{k\pi}, \\ d_2^2 < d_3^2 &\iff \theta > \frac{3\pi}{4} - \frac{2(a-b)(c-d)}{k\pi}. \end{aligned}$$

These inequalities are used in the characterization of all MSSR curves for Case (i) in which  $X, Y \in \mathcal{S}_{\text{top}}$ .

Case (i) has seven subcases: three in which there is a unique MSSR curves, three in which there are non-unique MSSR curves with multiplicity 2, and one in which there are non-unique MSSR curves with multiplicity 3. We denote these cases by either  $d_i$ ,  $d_i = d_j$  or  $d_1 = d_2 = d_3$ . In the case denoted by  $d_i$ , the MSSR curve from  $X$  to  $Y$  is unique, has length  $d_{\mathcal{SR}}(X, Y) = d_i$ , and corresponds to the minimal pair  $((U, D), (V_i, \Lambda_i))$  using (2). In the case denoted  $d_i = d_j$ , there are exactly two MSSR curves from  $X$  to  $Y$ , of length  $d_{\mathcal{SR}}(X, Y) = d_i = d_j$ , and corresponding to the minimal pairs  $((U, D), (V_i, \Lambda_i))$  and  $((U, D), (V_j, \Lambda_j))$ . The notation for the last case with three MSSR curves is similarly understood.

The seven cases are distinguished by the relationship of the quantity  $m := \frac{2(a-b)(c-d)}{k\pi}$  and the angle  $\theta$ . Denote . If  $m > \min(\theta, \pi - \theta) - \pi/4$ , then

$$d_{\mathcal{SR}}(X, Y) = \begin{cases} d_1, & \theta < \pi/2, \\ d_1 = d_2, & \theta = \pi/2, \\ d_2, & \theta > \pi/2. \end{cases}$$

If  $m = \min(\theta, \pi - \theta) - \pi/4$ , then

$$d_{\mathcal{SR}}(X, Y) = \begin{cases} d_1 = d_3, & \theta < \pi/2, \\ d_1 = d_2 = d_3, & \theta = \pi/2, \\ d_2 = d_3, & \theta > \pi/2. \end{cases}$$

Finally, if  $m < \min(\theta, \pi - \theta) - \pi/4$ , then

$$d_{\mathcal{SR}}(X, Y) = d_3.$$

The conditions leading to these seven subcases are graphically summarized in Fig. 1.

The MSSR curves corresponding to cases  $d_1$  and  $d_2$  can be understood as the rotation and scaling of the ellipse corresponding to  $X$  to the ellipse corresponding to  $Y$ , where the rotation is either counterclockwise (case  $d_1$ ), or clockwise (case  $d_2$ ). In these two subcases, the whole MSSR curve never leaves the distinct eigenvalue subset of  $\text{Sym}^+(2)$  (the top stratum). On the other hand, the MSSR curves corresponding to “ $d_3$ ” always pass through the equal-eigenvalue subset of  $\text{Sym}^+(2)$  (the bottom stratum). The direction of rotation for  $d_3$  depends on  $\theta$ : counterclockwise if  $\theta < \pi/2$ , clockwise if  $\theta > \pi/2$ . (There is no rotation if  $\theta = \pi/2$ .)

These seven subcases are illustrated by representative examples in Figs. 2–8. If  $d_1$  and  $d_2$  are thought of as the same “type”, then there are five different types of (non-)uniqueness behavior of MSSR curves in Case (i), as follows:

1. Unique MSSR curve (completely contained in the distinct eigenvalue subset), if  $m > \min(\theta, \pi - \theta) - \pi/4$  and  $\theta \neq \pi/2$ . Cases  $d_1$  (Fig. 2) and  $d_2$  (Fig. 3) are of this type.
2. Unique MSSR curve (leaving the distinct eigenvalue subset and passing through the bottom stratum), if  $m < \min(\theta, \pi - \theta) - \pi/4$ . Case  $d_3$  (Fig. 4) is of this type.
3. Two MSSR curves with rotation angle  $\pi/2$  (still completely contained in the distinct eigenvalue subset), if  $m > \min(\theta, \pi - \theta) - \pi/4$  and  $\theta = \pi/2$ . Case  $d_1 = d_2$  (Fig. 5) is of this type.
4. Two MSSR curves (one in the distinct eigenvalue subset, the other passing through the bottom stratum), if  $m = \min(\theta, \pi - \theta) - \pi/4$  and  $\theta \neq \pi/2$ . Cases  $d_1 = d_3$  (Fig. 6) and  $d_2 = d_3$  (Fig. 7) are of this type.
5. Three MSSR curves (two with rotation angle  $\pi/2$ , completely contained in the distinct eigenvalue subset, and the other involving no rotation but passing through the bottom stratum), if  $m = \min(\theta, \pi - \theta) - \pi/4$  and  $\theta = \pi/2$ . Case  $d_1 = d_2 = d_3$  (Fig. 8) is of this type.

For each given  $X$  and  $Y$ , if one takes  $k$  small enough that  $m > \pi/4$ , then MSSR curves from  $X$  to  $Y$  are always of type  $d_1$  or  $d_2$ . In other words, if  $k$  is small enough (for fixed  $X, Y$ ), the MSSR curve(s) are completely contained in the distinct eigenvalue subset.

**Case (ii).** ( $a = b$  and  $c \geq d$ ) By Theorem 4.1 of [1], the MSSR curve from  $X$  to  $Y$  is unique, and is

$$\chi(t) = (UR_\theta) \exp \begin{pmatrix} (1-t)a + tc & 0 \\ 0 & (1-t)a + td \end{pmatrix} (UR_\theta)^T,$$

and  $d_{\mathcal{SR}}(X, Y) = \sqrt{(a-c)^2 + (a-d)^2}$ . If in addition  $c = d$ , then  $\chi(t) = e^{(1-t)a+tc} I_2$ .

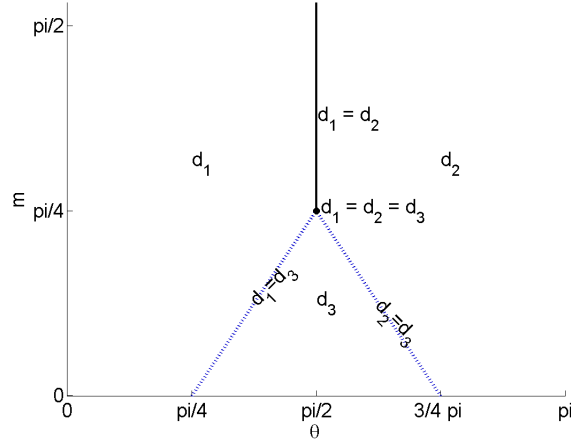


FIG 1. Unique and non-unique MSSR curves in  $\text{Sym}^+(2)$ : Schematic illustration for the seven subcases of Case (i) in which both  $X$  and  $Y$  are in  $S_{\text{top}}$ .

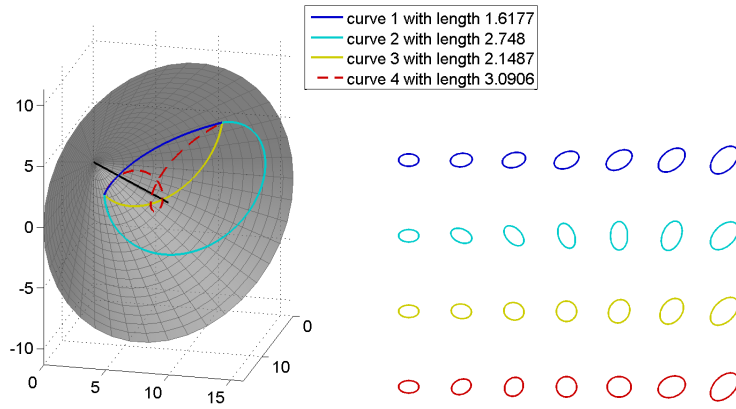
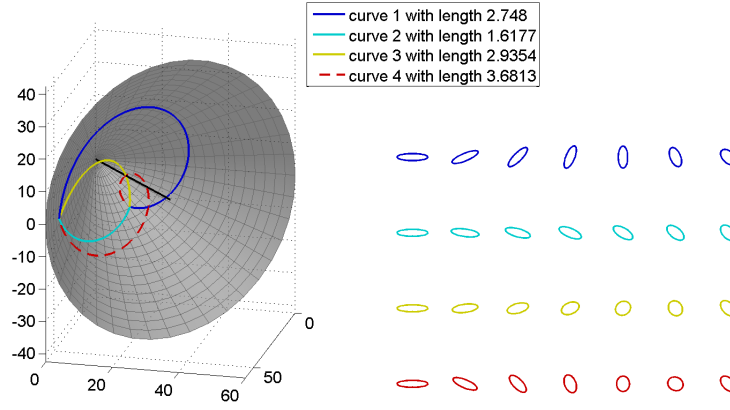
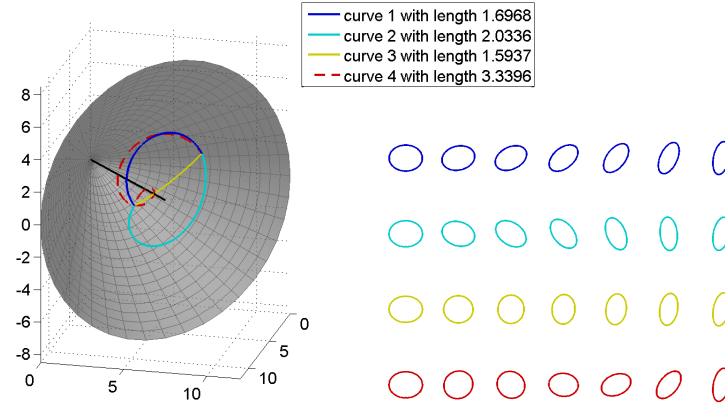
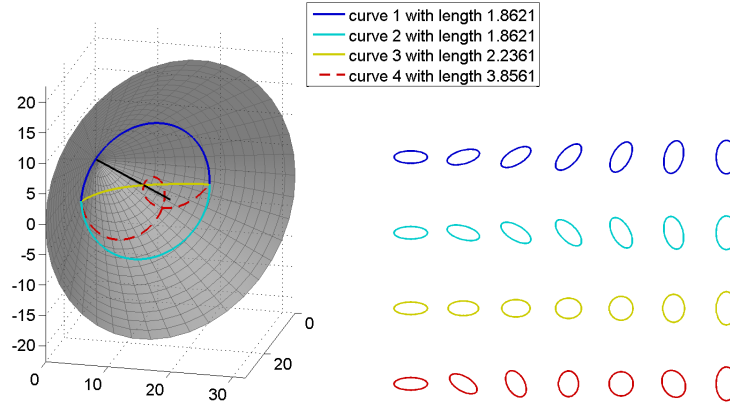
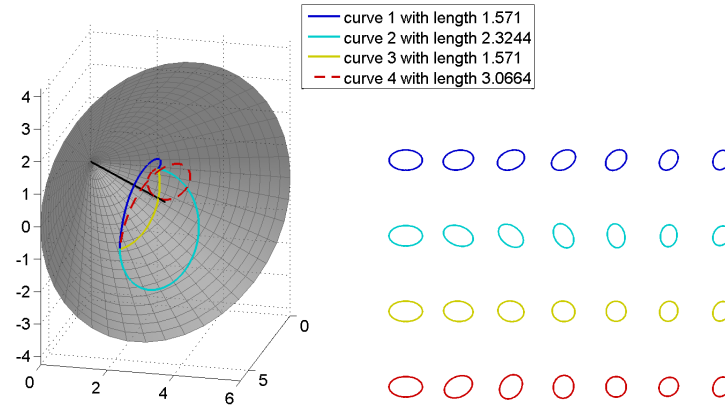
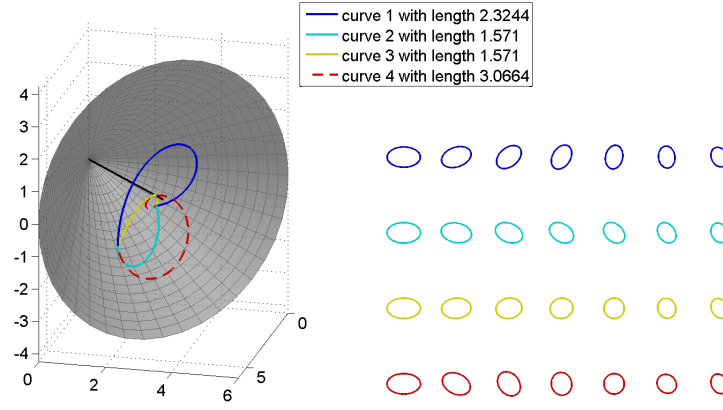
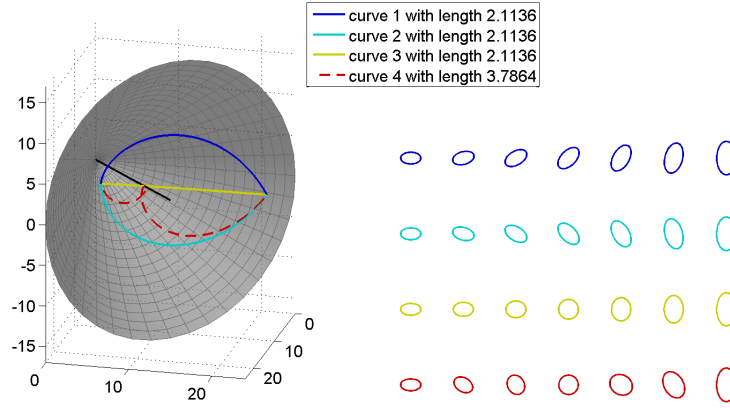


FIG 2. An example for subcase  $d_1$ . For each  $i = 1, 2, 3, 4$ , “curve  $i$ ” represents the scaling-rotation curve corresponding to the pair  $((U, D), (V_i, \Lambda_i))$ , and whose length is  $d_i$ .  $\text{Sym}^+(2)$  is an open cone in the three-dimensional space  $\text{Sym}(2)$ . The black line is the axis of the cone. Each curve, labeled by the same color in the left and right panels, is illustrated as the space curve  $\chi(t)$ , contained in this cone  $\text{Sym}^+(2)$  (left), or as the sequence of corresponding ellipses (right). In this and all other examples, the scaling factor  $k$  is set equal to 1.

FIG 3. An example for subcase  $d_2$ .FIG 4. An example for subcase  $d_3$ .

FIG 5. An example for subcase  $d_1 = d_2$ .FIG 6. An example for subcase  $d_1 = d_3$ .

FIG 7. An example for subcase  $d_2 = d_3$ .FIG 8. An example for subcase  $d_1 = d_2 = d_3$ .

## 2. Scaling-rotation distance and MSSR curves in $\text{Sym}^+(3)$

In the section, we give examples, graphical illustrations, and further discussion of unique and non-unique cases of MSSR curves in  $\text{Sym}^+(3)$ . As shown in Theorem 4.4 of the main article, we can divide our analysis into four possibilities for the strata in which  $X$  and  $Y$  lie.

- (i)  $X, Y \in \mathcal{S}_{\text{top}}$ .
- (ii)  $X \in \mathcal{S}_{\text{mid}}, Y \in \mathcal{S}_{\text{top}}$ .
- (iii)  $X, Y \in \mathcal{S}_{\text{mid}}$ .
- (iv)  $X \in \mathcal{S}_{\text{bot}}$ .

The case (i) in which both  $X$  and  $Y$  have three distinct eigenvalues is discussed in Section 2.1. For cases (ii) and (iii), graphical illustrations and further discussion of all classes of MSSR curves are provided in Section 2.2 for case (ii), and in Section 2.3 for case (iii) with reference to Section 5 of the main article. It is easy to see that in the case (iv) there is a unique MSSR curve for any  $Y \in \text{Sym}^+(3)$ .

### 2.1. The case in which both $X$ and $Y$ have three distinct eigenvalues

Let  $X, Y \in \mathcal{S}_{\text{top}} := \mathcal{S}_{[\text{J}_{\text{top}}]}$ , and let  $(U, D) \in \mathcal{E}_X, (V, \Lambda) \in \mathcal{E}_Y$ . By Proposition 3.7 (of the main article),  $((U, D), (VP_g^{-1}, \pi_g \cdot \Lambda))$  is a minimal pair if  $g$  is in the set

$$N_{((U,D),(V,\Lambda))} = \underset{g \in \tilde{S}_3^+}{\text{argmin}} \left\{ kd_{SO(3)}^2(U, VP_g^{-1}) + d_{\mathcal{D}}^2(D, \pi_g \cdot \Lambda) \right\}. \quad (3)$$

Depending on  $(U, D), (V, \Lambda)$ , any  $g \in \tilde{S}_3^+$  can provide a minimal pair. Let  $n_{(X,Y)} := |N_{((U,D),(V,\Lambda))}|$ , which is insensitive to particular choices of  $((U, D), (V, \Lambda))$ . If  $n_{(X,Y)} = 1$ , then the MSSR curve from  $X$  to  $Y$  is unique; if  $n_{(X,Y)} > 1$ , then there are just  $n_{(X,Y)}$  MSSR curves.

Given a particular pair  $((U, D), (V, \Lambda))$ , the 24 elements of  $\tilde{S}_3^+$  label the corresponding scaling-rotation curves, which are candidates for the MSSR curves. A strategy to characterize all unique and non-unique cases of MSSR curves is to divide the minimization problem into smaller subproblems. To this end, we classify these subproblems according to the six values of  $\text{proj}_2(g) = \pi_g \in S_3$ . Recall that we write  $\pi_{\text{id}}$  for the identity permutation, and, for distinct  $a, b \in \{1, 2, 3\}$ , we write  $\pi_{ab}$  for the transposition  $(ab)$ , the permutation that just interchanges  $a$  and  $b$ . All six elements of  $S_3$  are

$$\begin{aligned} &\pi_{\text{id}}, \\ &\pi_{12}, \quad \pi_{23}, \\ &\pi_{123} := \pi_{23}\pi_{12}, \quad \pi_{132} := \pi_{12}\pi_{23}, \\ &\pi_{13} (= \pi_{12}\pi_{23}\pi_{12} = \pi_{23}\pi_{12}\pi_{23}). \end{aligned} \quad (4)$$

Within the set of  $g$ 's projecting to each permutation  $\pi_\star \in S_3$ , we can find  $X, Y$  such that there are unique or non-unique  $g$ 's that give the smallest distance. The

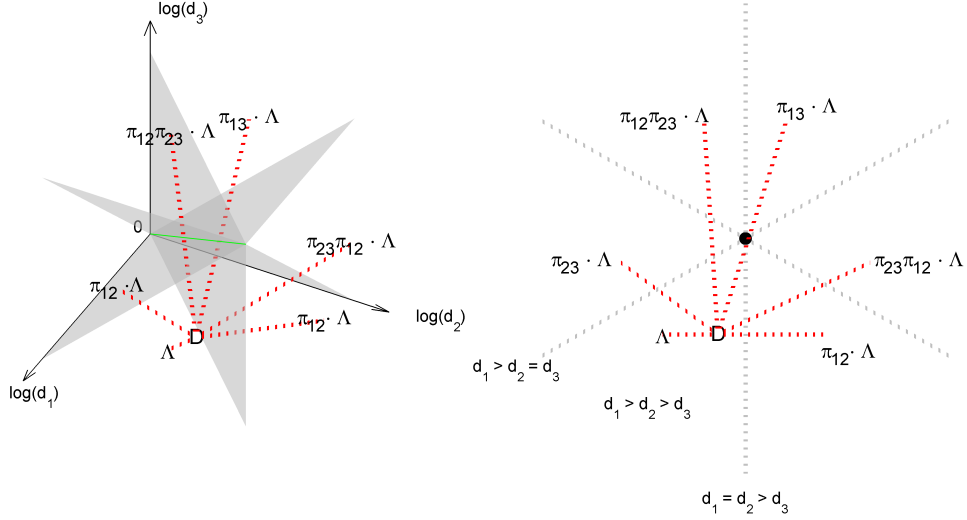


FIG 9. The space  $\text{Diag}^+(3)$  with the line and planes representing the its stratification (left) and a cross section (right) of the stratified  $\text{Diag}^+(3)$ ; see Fig. 3 of the main article. For  $D, \Lambda$  in the same connected component of  $\mathcal{D}_{\text{Jtop}} \subset \text{Diag}^+(3)$ , the distance  $d_{\mathcal{D}}(D, \Lambda)$  is represented by the “length” of the red dotted line. Also shown are  $\pi_g \cdot \Lambda$  and  $d_{\mathcal{D}}(D, \pi_g \cdot \Lambda)$  for all possible  $\pi_g$ . Here, we chose  $D = \text{diag}(8, 6, 3)$ ,  $\Lambda = \text{diag}(15, 8, 6)$ .

subproblem for each  $\pi_*$  has many subcases. For example, among the four  $g$ ’s with  $\pi_g = \pi_{\text{id}}$ , there are 8 subcases of (possibly) unique or non-unique MSSR curves, determined by the value of  $U^{-1}V$ . Instead of analyzing all subcases, we focus on the classification by the values of  $\pi_g$ , which provides interesting information concerning the corresponding MSSR curves.

For this purpose, we assume that  $D$  and  $\Lambda$  are in the same connected components of  $\mathcal{D}_{\text{Jtop}}$  (e.g.,  $d_1 > d_2 > d_3$  and  $\lambda_1 > \lambda_2 > \lambda_3$ ), so that the minimum of  $d_{\mathcal{D}}(D, \pi_g \cdot \Lambda)$  is achieved by choosing  $g$  to satisfy  $\pi_g = \pi_{\text{id}}$ . Moreover, if  $D$  and  $\Lambda$  satisfy  $d_1 > d_2 > d_3$ ,  $\lambda_1 > \lambda_2 > \lambda_3$ , then

$$d_{\mathcal{D}}(D, \pi_{\text{id}} \cdot \Lambda) \leq \left\{ \begin{array}{c} d_{\mathcal{D}}(D, \pi_{12} \cdot \Lambda) \\ \text{or} \\ d_{\mathcal{D}}(D, \pi_{23} \cdot \Lambda) \end{array} \right\} \leq \left\{ \begin{array}{c} d_{\mathcal{D}}(D, \pi_{123} \cdot \Lambda) \\ \text{or} \\ d_{\mathcal{D}}(D, \pi_{132} \cdot \Lambda) \end{array} \right\} \leq d_{\mathcal{D}}(D, \pi_{13} \cdot \Lambda).$$

In order for a  $g$  such that  $\pi_g \neq \pi_{\text{id}}$  to give a minimal pair, the corresponding “rotation distance” (the first term of (3)) needs to be much smaller than the four rotation distances associated with the identity permutation. A typical example of the distances  $d_{\mathcal{D}}(D, \pi_g \cdot \Lambda)$  is illustrated in Fig. 9.

In this example, because  $\pi_g = \pi_{\text{id}}$  gives the smallest  $d_{\mathcal{D}}(D, \pi_g \cdot \Lambda)$ , for sufficiently small  $k$  the minimizer  $g$  of (3) satisfies  $\pi_g = \pi_{\text{id}}$ . In this case the ellipsoids corresponding to the MSSR curves from  $t = 0$  to 1 are always tri-axial. For fixed  $k$ , other choices of  $g$  can provide a minimal pair, depending on the values of  $(U, D)$ ,  $(V, \Lambda)$ . Below, we list the shape-classification changes of the MSSR curve  $\chi_g$  corresponding to the particular  $g \in \mathbb{N}_{((U,D),(V,\Lambda))} \subset \tilde{S}_3^+$ . A  $3 \times 3$



SPD matrix with eigenvalues  $a \geq b \geq c$  has the shape of a sphere if  $a = b = c$ , oblate spheroid (or oblate, for short) if  $a = b > c$ , prolate spheroid (or prolate) if  $a > b = c$ , or tri-axial ellipsoid (or tri-axial) if  $a > b > c$ . We assume below that  $D$  and  $\Lambda$  have been chosen to lie in the same connected component of  $\mathcal{D}_{\text{Jtop}}$ .

1. For all  $g$  such that  $\pi_g = \pi_{\text{id}}$ , for all  $t \in [0, 1]$ , the ellipsoid corresponding to  $\chi_g(t)$  is always tri-axial.
2. For all  $g$  such that  $\pi_g = \pi_{12}$ , the shape-classification changes of the MSSR curves  $\chi_g(t)$  from  $t = 0$  to  $t = 1$  are (tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial).
3. For all  $g$  such that  $\pi_g = \pi_{23}$ , the shape-classification changes are (tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial).
4. For all  $g$  such that  $\pi_g = \pi_{123}$ , the shape-classification changes are (tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial).
5. For all  $g$  such that  $\pi_g = \pi_{132}$ , the shape-classification changes are (tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial).
6. For all  $g$  such that  $\pi_g = \pi_{13}$ , the shape-classification changes are either (tri-ax.  $\rightarrow$  oblate  $\rightarrow$  tri-ax.  $\rightarrow$  prolate  $\rightarrow$  tri-ax.  $\rightarrow$  oblate  $\rightarrow$  tri-ax.), (tri-ax.  $\rightarrow$  prolate  $\rightarrow$  tri-ax.  $\rightarrow$  oblate  $\rightarrow$  tri-ax.  $\rightarrow$  prolate  $\rightarrow$  tri-ax.), or (tri-axial  $\rightarrow$  sphere  $\rightarrow$  tri-axial).

We close this section by providing the worst-case example of non-uniqueness we have found, in which there are 9 MSSR curves. We choose  $X = \text{diag}(e^a, e^b, e^c)$ , where  $c = 1$ ,  $b = c + \frac{7\sqrt{7}}{6\sqrt{8}}\pi$ ,  $a = b + \sqrt{\frac{7}{72}}\pi$ , and  $Y = R\text{diag}(e^x, e^y, e^z)R^T$  where  $\phi^{-1}(R) = \frac{\pm 1}{2}(1 + i + j + k)$  and  $z = 0$ ,  $y = \frac{1}{3\sqrt{14}}\pi$ ,  $x = y + \sqrt{\frac{7}{72}}\pi$ . The nine MSSR curves are illustrated in Fig. 10. (See below for the definition of  $\phi^{-1}(R)$ .)

## 2.2. The case in which $X \in \mathcal{S}_{\text{mid}}$ and $Y \in \mathcal{S}_{\text{top}}$

For this special case,  $X$  has just two distinct eigenvalues, while  $Y$  has three distinct eigenvalues. We parameterize  $X$  with  $a, b \in \mathbb{R}$  (arbitrary, not size-ordered), and any  $U \in \text{SO}(3)$ , and parameterize  $Y$  with  $c > d > f > 0$  and a unit quaternion  $q = z + wj \in S_{\mathbb{H}}^3$ , where  $z, w \in \mathbb{C}$  and,  $|z|^2 + |w|^2 = 1$ , as follows:

$$X = U \begin{pmatrix} e^a & 0 & 0 \\ 0 & e^b & 0 \\ 0 & 0 & e^b \end{pmatrix} U^T, \quad Y = U\phi(q) \begin{pmatrix} e^c & 0 & 0 \\ 0 & e^d & 0 \\ 0 & 0 & e^f \end{pmatrix} (U\phi(q))^T \quad (5)$$

where  $\phi : S_{\mathbb{H}}^3 \rightarrow \text{SO}(3)$  is the natural two-to-one Lie-group homomorphism. Without loss of generality, we assume  $\text{Re}(q) = \text{Re}(z) > 0$  so that  $\phi(q)$  is not an involution.

There are six different cases of MSSR curves as summarized in Table 3 of the main article, named  $A_1, A_2, B_1, B_2, C_1, C_2$ . To give representative examples of these cases, we partially rewrite the conditions in Table 4 of the main article.

Recall that  $\varphi = \cos^{-1}(\max\{|z|, |w|\}) \in [0, \frac{\pi}{4}]$ . For each  $\varphi \in (0, \pi/4)$  there are exactly two cases:  $\cos(\varphi) = |z| > |w|$  and  $|z| < |w| = \cos(\varphi)$ . If  $\varphi = 0$ , then  $|z| = 1, |w| = 0$ . If  $\varphi = \frac{\pi}{4}$ , then  $|z| = |w| = 1/\sqrt{2}$ . The parameters  $\beta, \beta'$ ,

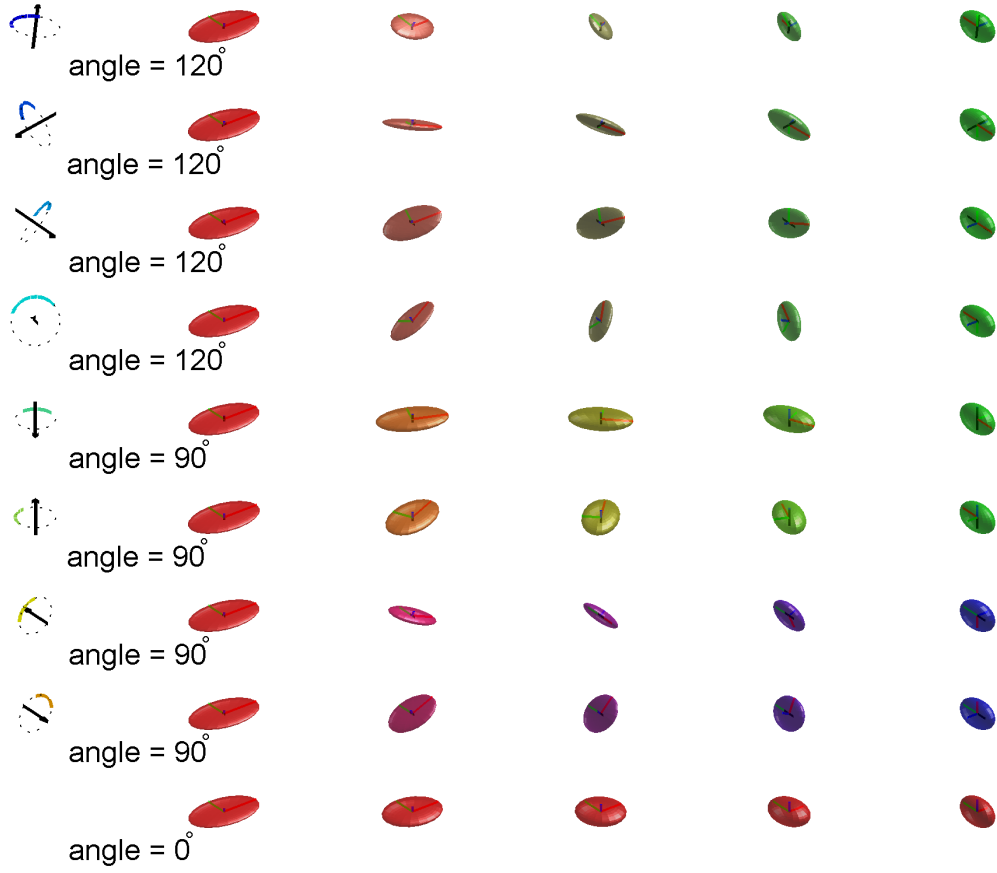


FIG 10. An example for one case of non-unique MSSR curves, where  $X, Y \in \mathcal{S}_{\text{top}}$ . There are nine MSSR curves. The rotation parameter  $A$  of each MSSR curve is depicted as the axis-angle figure in the left-most panels. The top four MSSR curves correspond to the minimal pairs provided by  $g$  with  $\pi_g = \pi_{\text{id}}$ . The next two MSSR curves correspond to two choices of  $g$  with  $\pi_g = \pi_{12}$ . The next two MSSR curves correspond to two choices of  $g$  with  $\pi_g = \pi_{23}$ . The last MSSR curve corresponds to  $g$  with  $\pi_g = \pi_{123}$ .

$\text{Re}(\bar{z}w)$ , and  $\text{Im}(\bar{z}w)$  appearing in Theorem 4.4 and Table 4 of the main article will be represented by

$$\alpha = \begin{cases} \cos^{-1} \left( \frac{|\text{Re}(\bar{z}w)|}{|\bar{z}w|} \right), & \text{if } \varphi > 0; \\ \pi/2, & \text{if } \varphi = 0. \end{cases} \in [0, \frac{\pi}{2}], \quad (6)$$

so that

$$\beta = \frac{1}{2} \cos^{-1}(\sin(2\varphi) \cos \alpha) \in [0, \frac{\pi}{4}], \quad (7)$$

$$\beta' = \frac{1}{2} \cos^{-1}(\sin(2\varphi) \sin \alpha) \in [0, \frac{\pi}{4}]. \quad (8)$$

Note that

$$\varphi = 0 \iff |z| = 1 \iff \beta = \beta' = \frac{\pi}{4} \quad (9)$$

and that

$$\operatorname{Re}(\bar{z}w) = 0 \iff \cos \alpha = 0 \iff \alpha = \frac{\pi}{2}, \quad (10)$$

$$\operatorname{Im}(\bar{z}w) = 0 \iff \cos \alpha = 1 \iff \alpha = 0. \quad (11)$$

For any  $\alpha < \pi/2$ ,  $\operatorname{Re}(\bar{z}w)$  can have either sign. For  $\alpha > 0$ ,  $\operatorname{Im}(\bar{z}w)$  can have either sign.

We also make use of the following parameters, concerning the scaling of eigenvalues:

$$m_1 = \frac{2(a-b)(c-d)}{4k}, \quad m_2 = \frac{2(a-b)(d-f)}{4k}. \quad (12)$$

Both  $m_1$  and  $m_2$  can be either positive or negative, but they must have the same sign. To simplify the analysis, we assume

$$m_1 = m_2 := m'. \quad (13)$$

Then we have

$$\ell_{\text{id}}^2 < \ell_{13}^2 \iff \varphi^2 - \beta^2 - 2m' < 0 \quad (14)$$

$$\ell_{\text{id}}^2 < \ell_{12}^2 \iff \varphi^2 - (\beta')^2 - m' < 0 \quad (15)$$

$$\ell_{13}^2 < \ell_{12}^2 \iff \beta^2 - (\beta')^2 + m' < 0 \quad (16)$$

By (7), (14) is equivalent to

$$\alpha > \cos^{-1} \left( \frac{\cos(2\sqrt{(\varphi^2 - 2m')_+})}{\sin(2\varphi)} \right), \quad \text{if } \varphi > 0,$$

and to  $m' > -\frac{\pi^2}{32}$  if  $\varphi = 0$ . By (8), (15) is equivalent to

$$\alpha < \sin^{-1} \left( \frac{\cos(2\sqrt{(\varphi^2 - m')_+})}{\sin(2\varphi)} \right), \quad \text{if } \varphi > 0,$$

and to  $m' > -\frac{\pi^2}{16}$  if  $\varphi = 0$ . We have not found a similarly simple inequality equivalent to (16). Using a numerical method, Fig. 11 provides the regions of

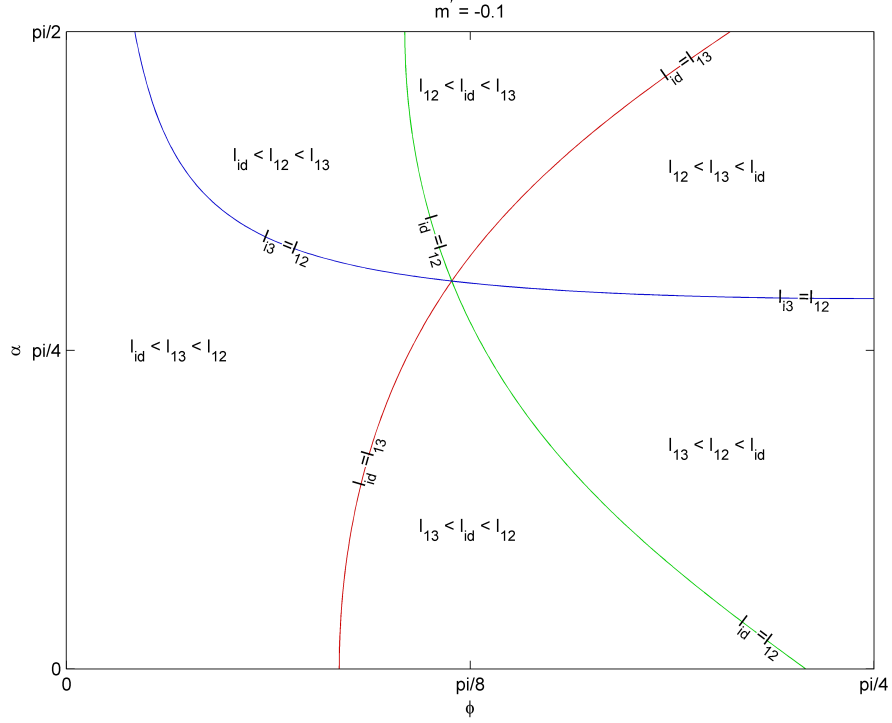


FIG 11. The order of  $\ell_{id}, \ell_{13}, \ell_{12}$  corresponding to the values of  $\varphi \in [0, \pi/4]$  and  $\alpha \in [0, \pi/2]$ . Note that  $m' = -0.1$  is fixed.

$(\varphi, \alpha)$  corresponding to different size-orders of  $\ell_{id}, \ell_{13}, \ell_{12}$ , for a fixed value of  $m' = -0.1$ . The seven cases of unique and non-unique MSSR curves summarized in Table 4 of the main article are graphically represented in Figs. 12 and 13.

In order to choose examples of  $(a, b, c, d, f)$  and  $q = z + wj$  for a given  $(m', \varphi, \alpha)$ , we use the following observations. If  $\varphi = 0$ , then  $q = 1$ . For a given  $\varphi \in (0, \pi/4]$ , write  $z = z_1 + z_2i$  and choose  $z_1$  such that  $0 < z_1 \leq \cos(\varphi)$ . Then,  $z_2 = \pm \sqrt{\cos(\varphi)^2 - z_1^2}$ , and in this case  $|z| \geq |w|$ . (The case  $|z| < |w|$  can be handled similarly.) We set  $w = e^{i\alpha} \sqrt{(1 - |z|^2)/|z|^2} z$ .

In the following we provide several examples of the unique and non-unique cases of MSSR curves for the case  $X \in \mathcal{S}_{\text{mid}}$  and  $Y \in \mathcal{S}_{\text{top}}$ . We first discuss the shape classification changes of the scaling-rotation curves  $\chi_{A_l}(t)$ ,  $\chi_{B_m}(t)$  and  $\chi_{C_n}(t)$  ( $l, m, n = 1, 2$ ). These depend on the sign of  $m'$ .

1. If  $m' > 0$  (that is,  $X$  is prolate, and  $Y$  is tri-axial), then the shape-classification changes of  $\chi_{A_l}(t)$  are (prolate  $\rightarrow$  tri-axial); for  $\chi_{B_m}(t)$  they are (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial); for  $\chi_{C_n}(t)$  they are (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial).
2. If  $m' < 0$  (that is,  $X$  is oblate, and  $Y$  is tri-axial), then the shape-classification changes of  $\chi_{A_l}(t)$  are (oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial); for  $\chi_{B_m}(t)$  they are (oblate  $\rightarrow$  tri-axial); for

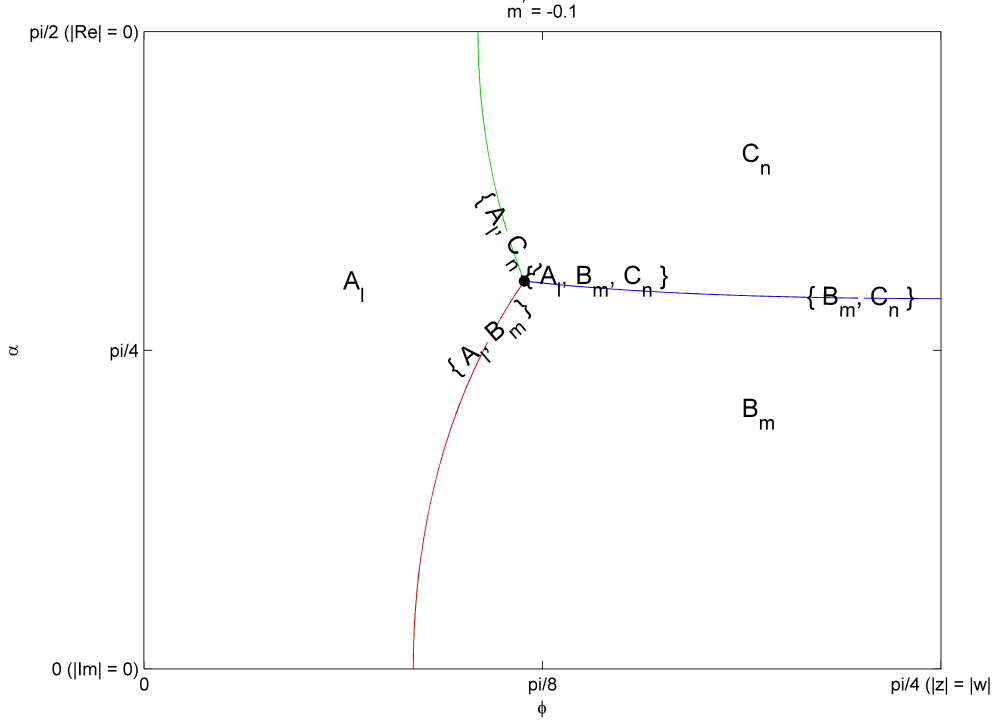


FIG 12. Cases of unique and non-unique MSSR curves in  $\text{Sym}^+(3)$  when  $X$  has just two distinct eigenvalues, and  $Y$  has three distinct eigenvalues. This figure uses the same parametrization of Fig. 11, with  $m' = -0.1$ . The case  $A_l$  stands for either  $A_1$  (if  $|z| > |w|$ ),  $A_2$  (if  $|z| < |w|$ ) or  $\{A_1, A_2\}$  (if  $|z| = |w|$ ). The latter case ( $|z| = |w|$ ) can only occur if  $\varphi = \pi/4$ . The case  $B_m$  stands for either  $B_1$  (if  $\text{Re}(\bar{z}w) > 0$ ),  $B_2$  (if  $\text{Re}(\bar{z}w) < 0$ ), or  $\{B_1, B_2\}$  (if  $\text{Re}(\bar{z}w) = 0$ ). The latter case ( $\text{Re}(\bar{z}w) = 0$ ) can only occur if  $\alpha = \pi/2$ . Similarly, the case  $C_n$  stands for either  $C_1$  (if  $\text{Im}(\bar{z}w) > 0$ ),  $C_2$  (if  $\text{Im}(\bar{z}w) < 0$ ), or  $\{C_1, C_2\}$  (if  $\text{Im}(\bar{z}w) = 0$ ). The latter case ( $\text{Im}(\bar{z}w) = 0$ ) can only occur if  $\alpha = 0$ . The multi-element cases such as  $\{A_l, B_m\}$  can be understood similarly. The values of  $l$  and  $m$  are determined by the signs of  $|z| - |w|$  and  $\text{Re}(\bar{z}w)$ , and if there are two values for  $l$  and one value for  $m$ , then the case is  $\{A_1, A_2, B_m\}$ , a case with three MSSR curves.

$\chi_{C_n}(t)$  they are (oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial).

Two scaling-rotation curves  $A_1$  and  $A_2$  (or  $B_1$  and  $B_2$ ,  $C_1$  and  $C_2$ ) share the same scaling parameters, and also share the same rotation axis, but with different orientations (one clockwise, the other counterclockwise) and possibly different angles. The two angles differ by  $\pi$ .

In an attempt to visually illustrate examples in Fig. 14 to Fig. 24, a scaling-rotation curve  $\chi := \chi_{U,D,A,L}$  in the 6-dimensional space  $\text{Sym}^+(3)$  is depicted by either a sequence of ellipsoids, representing the discretized scaling-rotation curve  $\chi$ , or the combination of the rotation parameter  $A$  and changes of eigenvalues  $D \exp(Lt)$ . The rotation parameters  $A$  of  $\chi$  are depicted as the axis-angle figure in the top left-most panels of figures below. The bottom panel of each figure depicts a logarithmic projection to  $\text{Diag}(3)$  of the curve  $D \exp(Lt) \in \text{Diag}^+(3)$

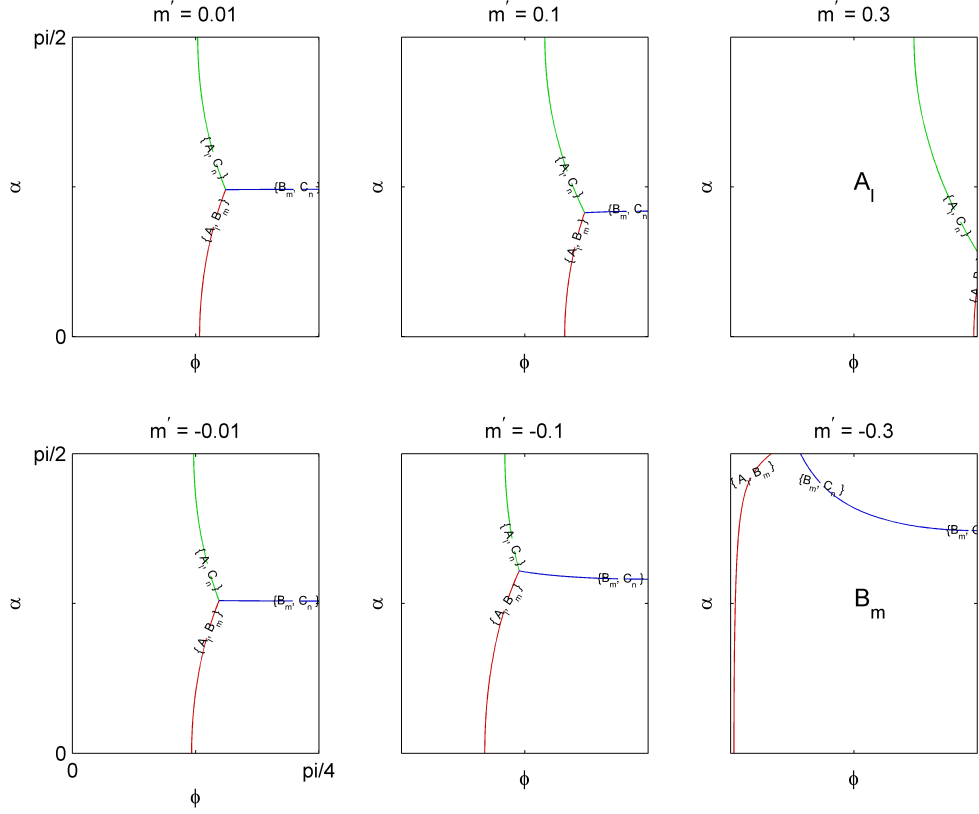


FIG 13. Unique and non-unique MSSR curves in  $\text{Sym}^+(3)$  when  $X$  has just two distinct eigenvalues, and  $Y$  has three distinct eigenvalues. As  $|m'|$  increases, either  $A_1$  or  $C_n$  becomes the only case of MSSR curves.

from  $D$  (black dot) to  $D \exp(L)$  (red dots). For  $(d_1, d_2, d_3) \in \text{Diag}^+(3)$ , each of the three shaded planes represents  $d_i = d_j$ ,  $(i \neq j)$ . The intersection of all shaded planes is the line  $d_1 = d_2 = d_3$  (black line), corresponding to  $\mathcal{D}_{\text{bot}}$  (or  $\mathcal{D}_{J_{\text{bot}}}$  with  $J_{\text{bot}} = \{\{1, 2, 3\}\}$ ). Each shaded plane, minus the black line, corresponds to  $\mathcal{D}_{J_i}$ , where  $J_1 = \{\{2, 3\}, \{1\}\}$ ,  $J_2 = \{\{1, 3\}, \{2\}\}$ ,  $J_3 = \{\{1, 2\}, \{3\}\}$ . The complement of the union of all three shaded planes corresponds to  $\mathcal{D}_{\text{top}} := \mathcal{D}_{J_{\text{top}}}$ . Since the rotational degrees of freedom have been projected out in the bottom panel, the relative lengths of the straight-line segments do not accurately reflect the relative lengths of the curves.

We collect representative visual examples of the unique MSSR curves in Figs 14, 15, 17 and 16. Cases where there are just two MSSR curves are illustrated in Figs. 18, 19, 20, 21 and 22. Cases where there are exactly three MSSR curves are illustrated in Figs. 23 and Figs. 24. More situations, including a four-MSSR curve case, are possible.

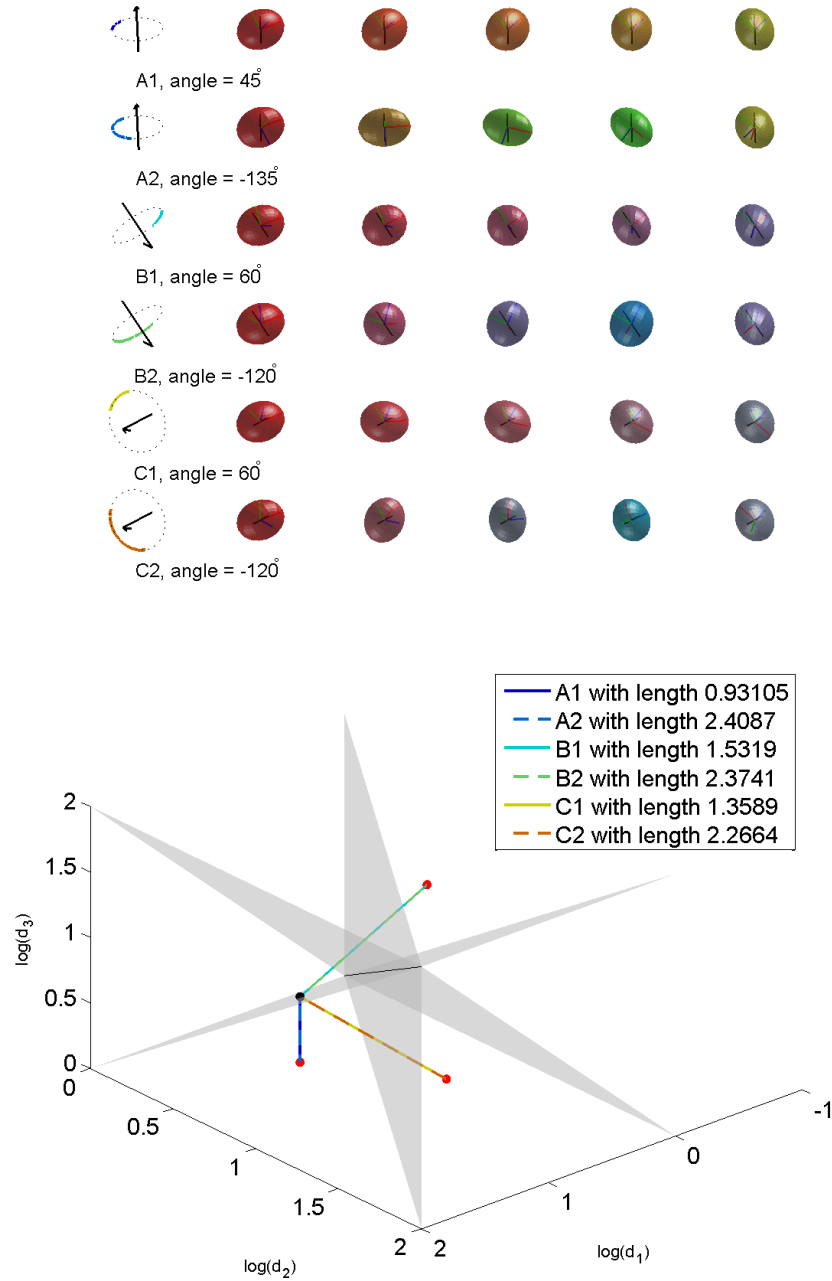


FIG 14. An example for the case  $\{A_1\}$ . (The scaling-rotation curve corresponding to  $A_1$  is the unique MSSR curve.) Each of the cases  $A_1 - C_2$  represents the corresponding scaling-rotation curve defined in Table 3 of the main article, whose length can be found in the legend. Note that  $m' > 0$  in this example. The eigenvalue paths corresponding to  $A_1$  and  $A_2$  depart from a single connected component of  $\mathcal{D}_{J_1}$  (represented by the shaded open half-plane containing the black dot) and reach  $\mathcal{D}_{\text{top}}$ . Accordingly, the shape-classification changes are (prolate  $\rightarrow$  tri-axial).

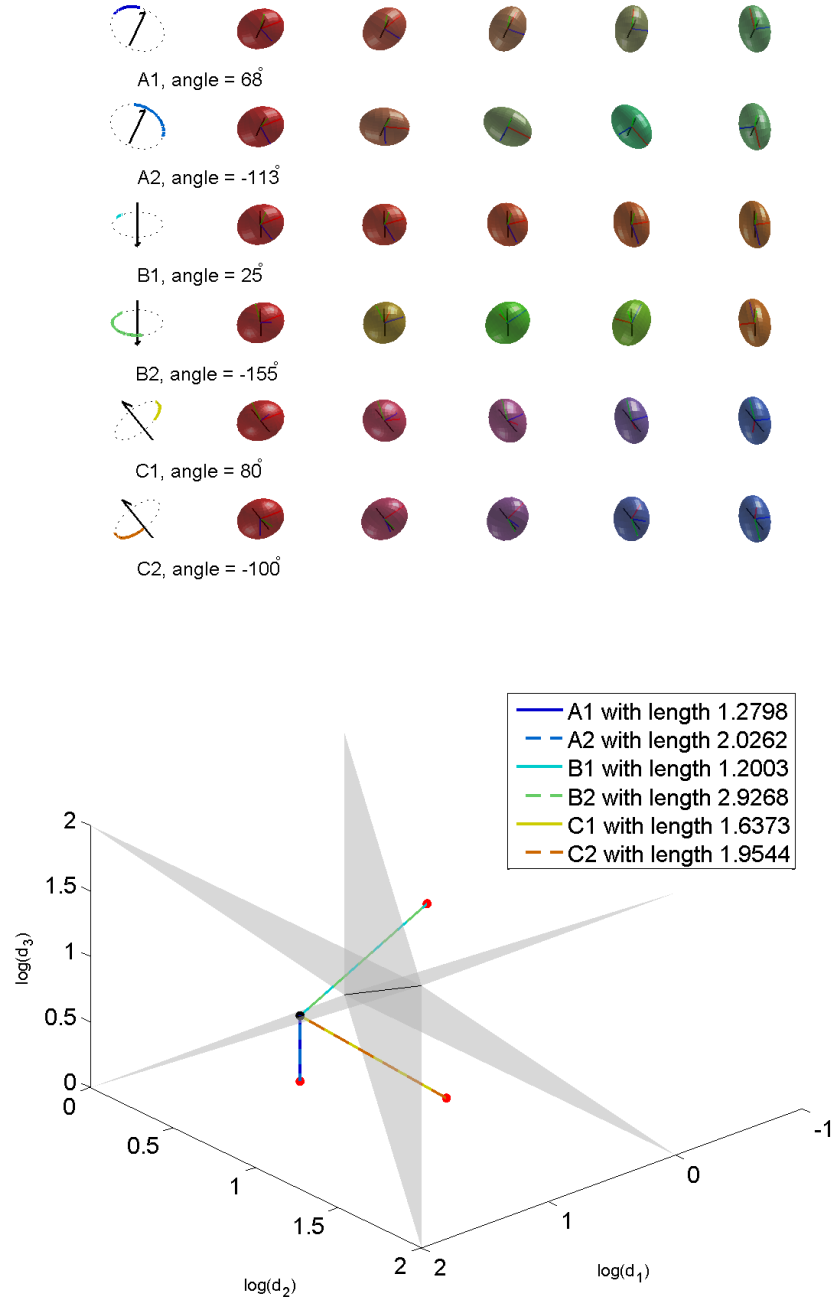


FIG 15. An example for the case  $\{B_1\}$ . In this example,  $m' > 0$ , and the shape-classification changes are (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate  $\rightarrow$  tri-axial).



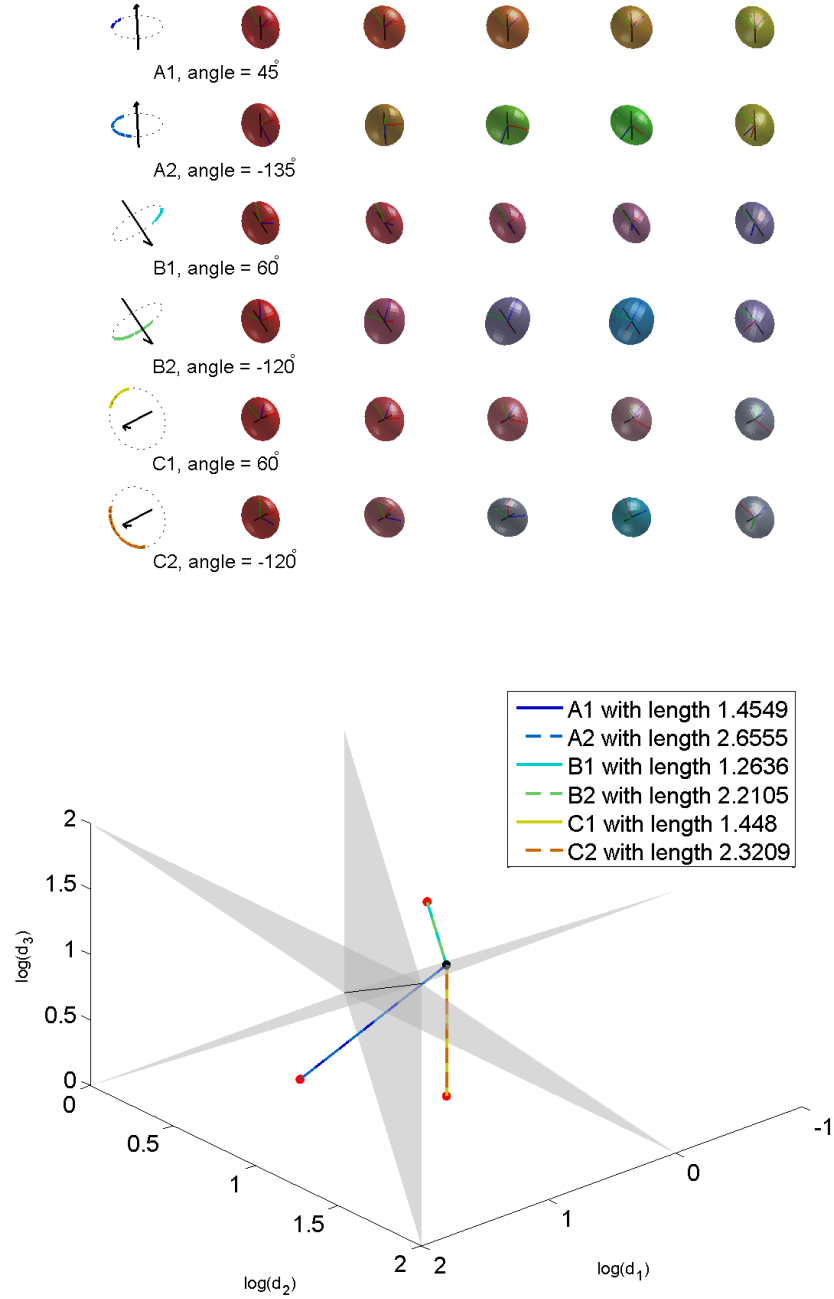
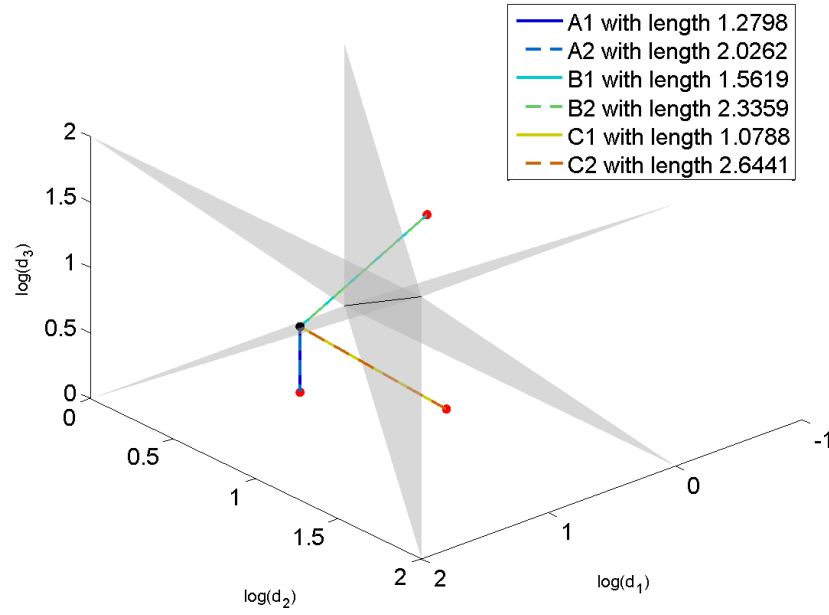
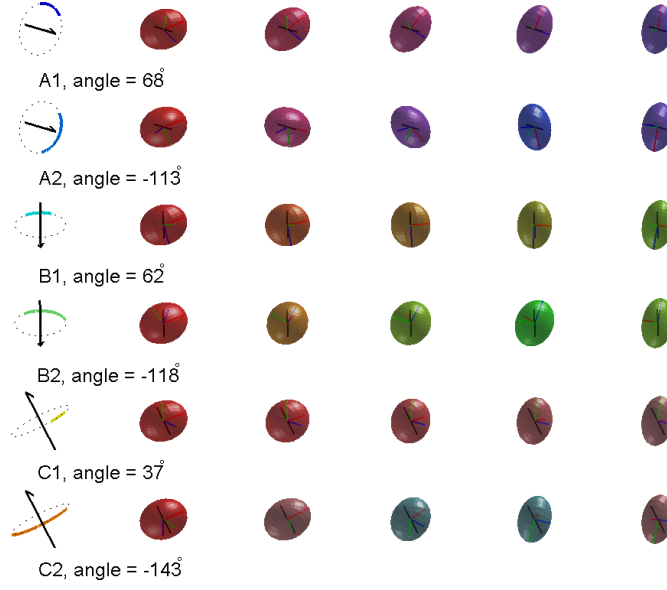
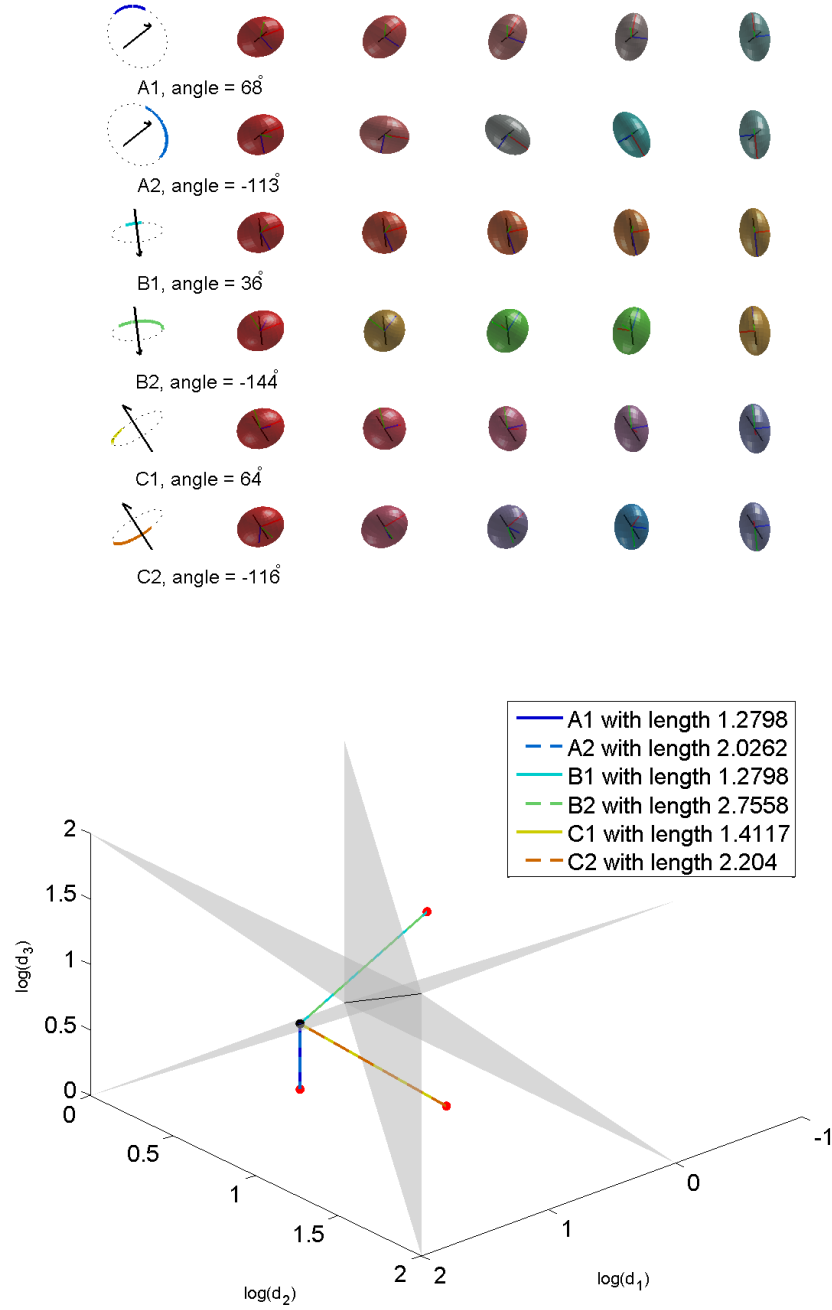
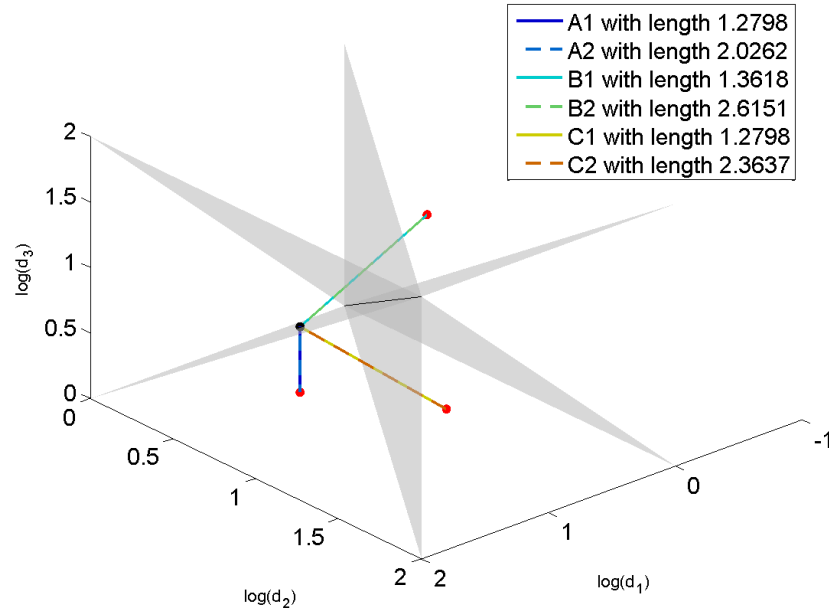
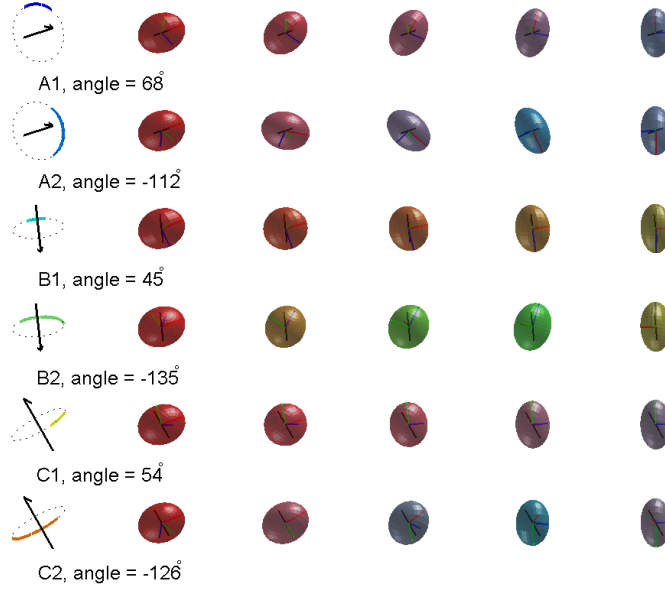
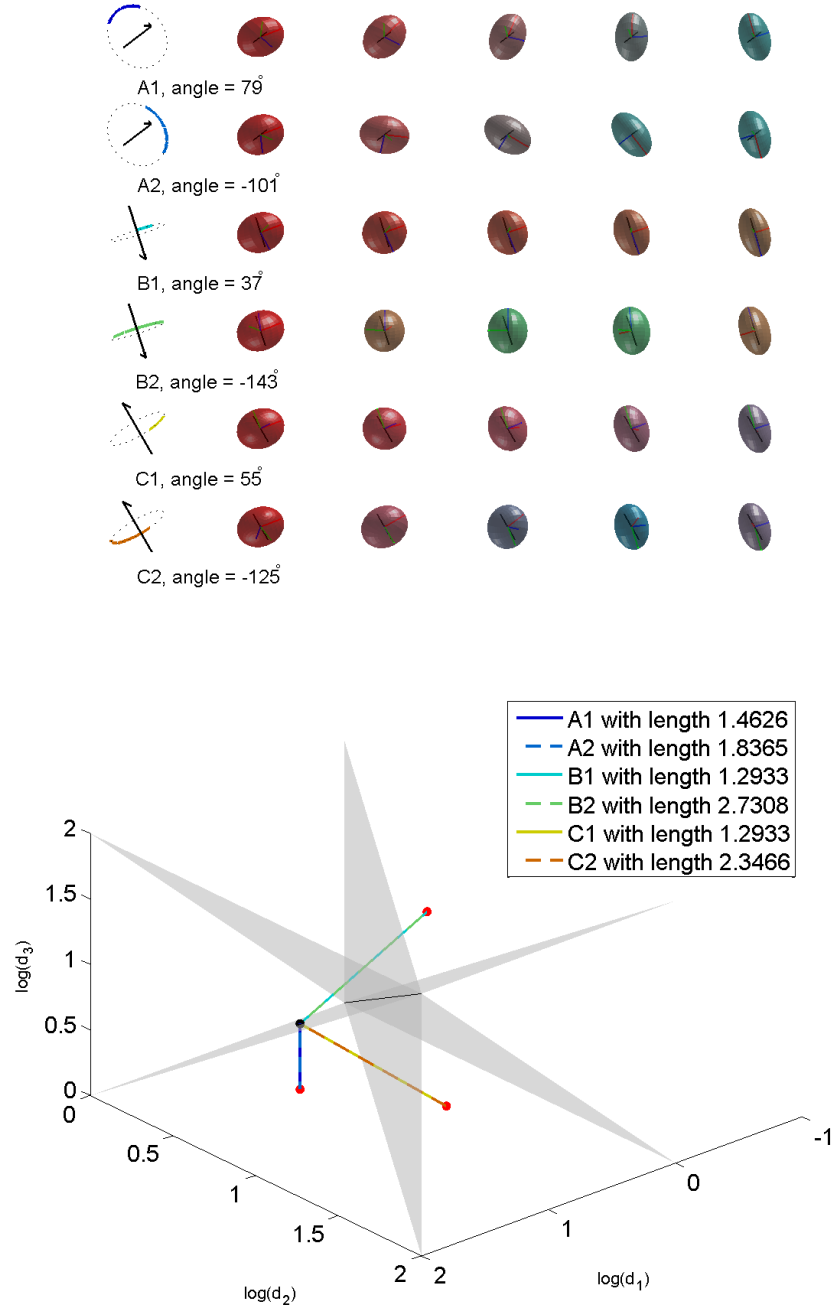


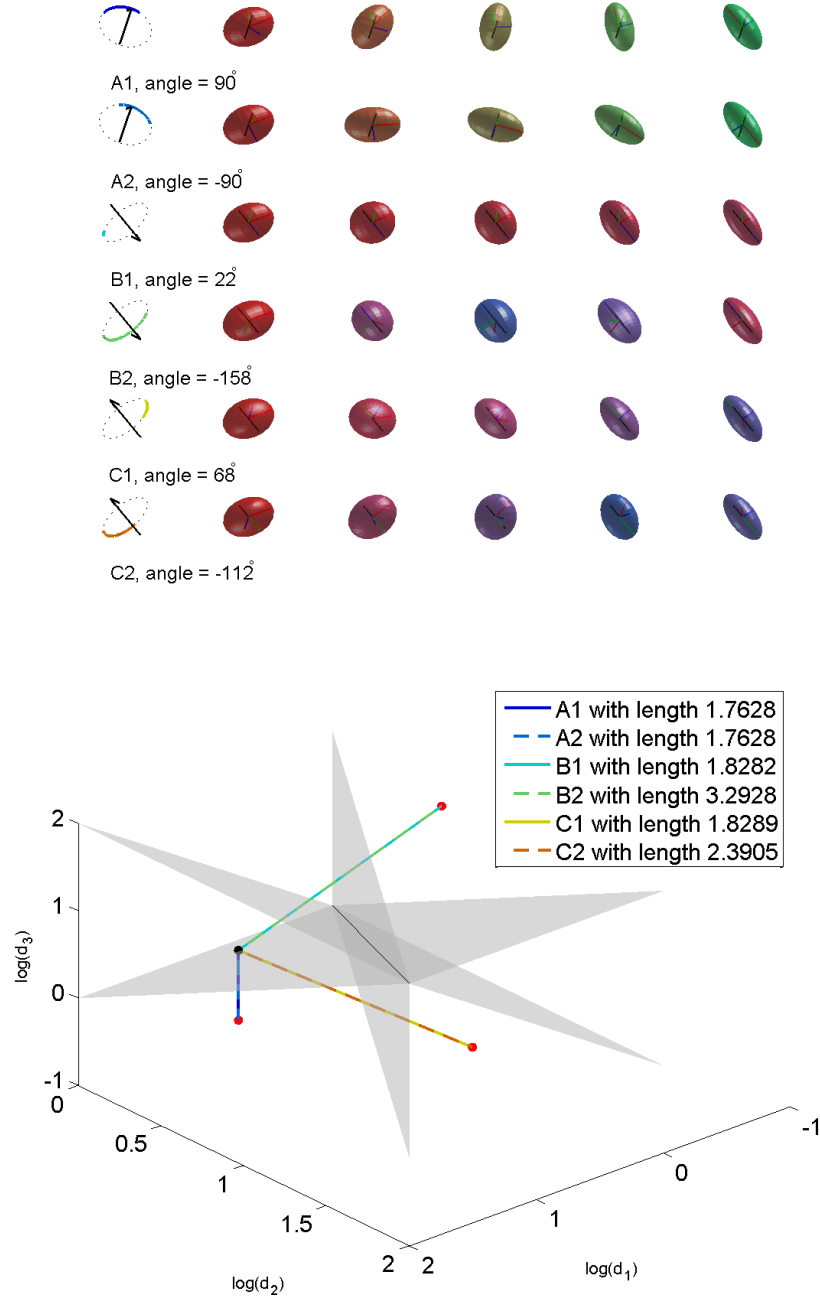
FIG 16. Another example for the case  $\{B_1\}$ , but with  $m' < 0$ . The shape-classification changes are (oblate  $\rightarrow$  tri-axial).

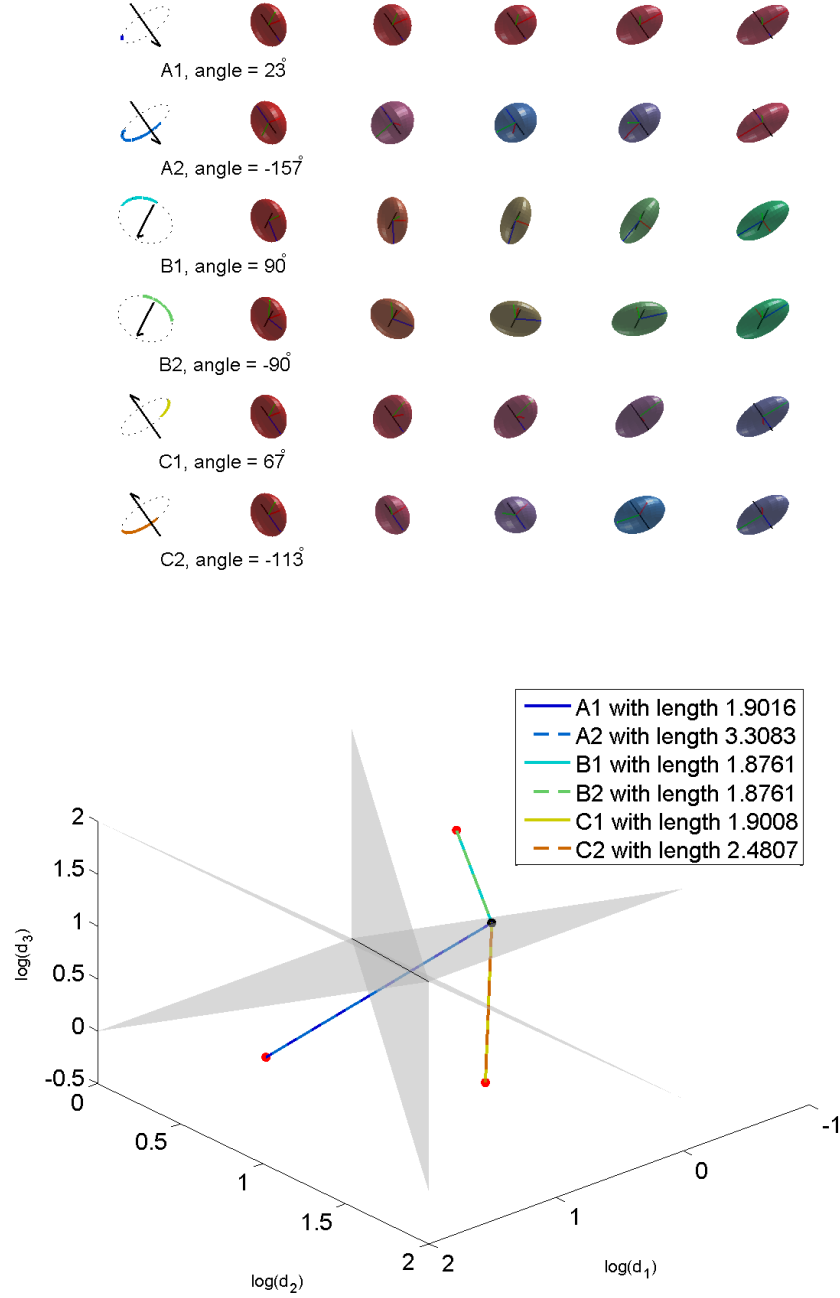
FIG 17. An example for the case  $\{C_1\}$ .

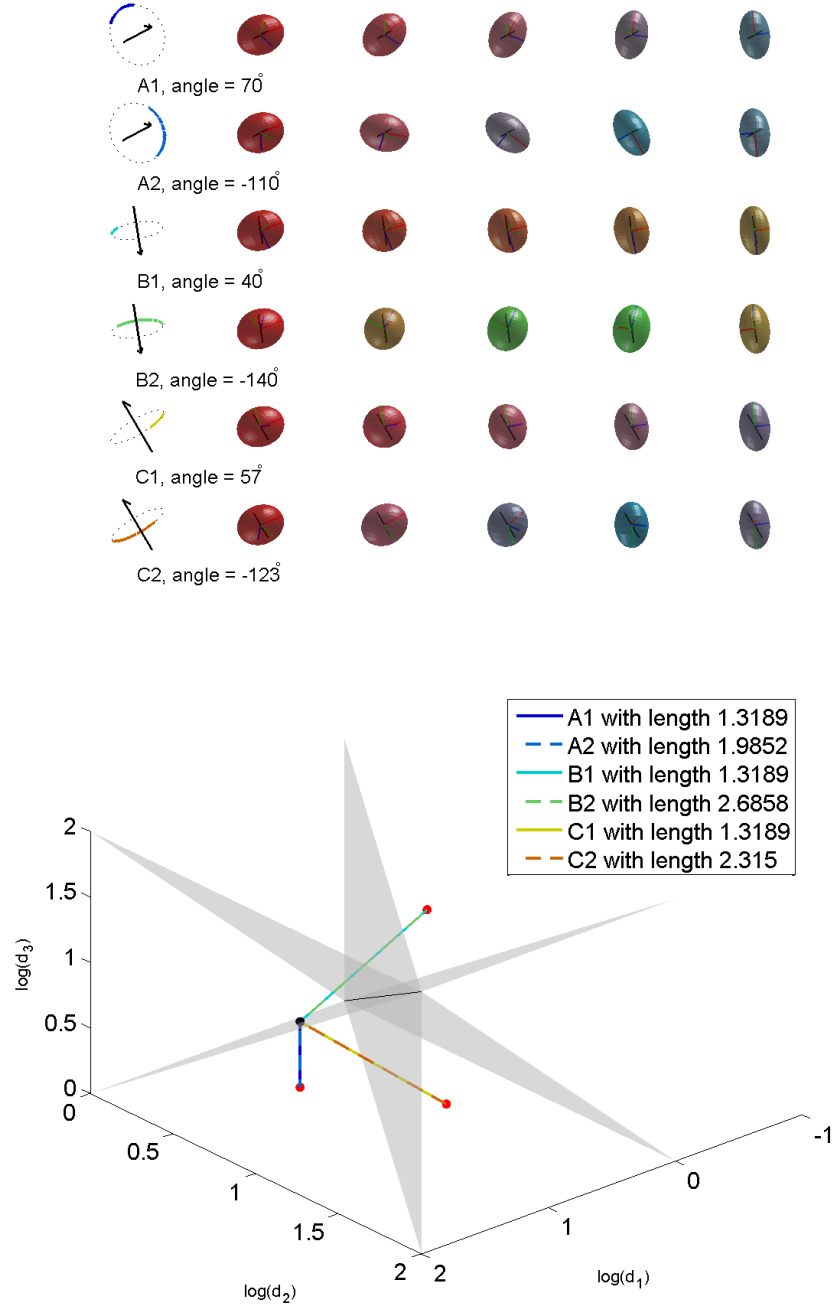
FIG 18. An example for the case  $\{A_1, B_1\}$ .

FIG 19. An example for the case  $\{A_1, C_1\}$ .

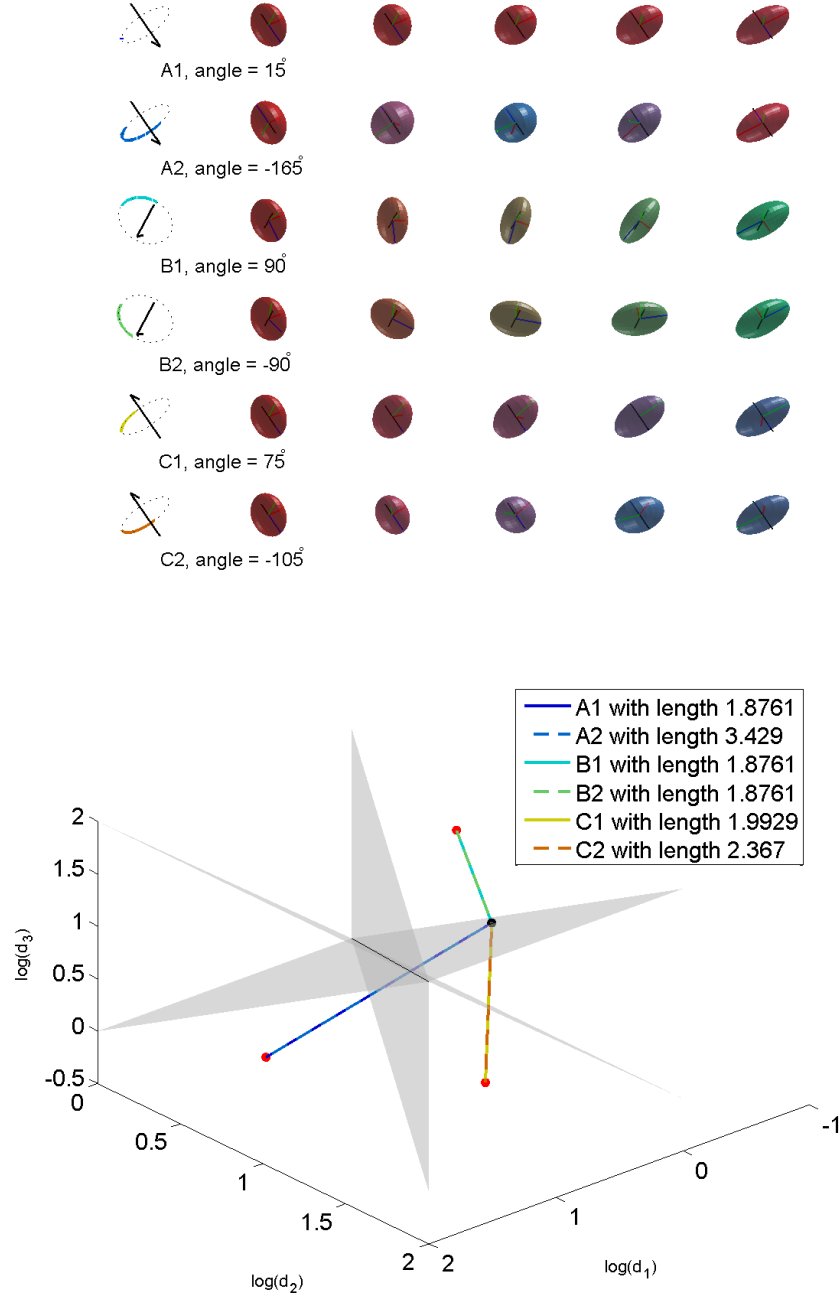
FIG 20. An example for the case  $\{B_1, C_1\}$ .

FIG 21. An example for the case  $\{A_1, A_2\}$ .

FIG 22. An example for the case  $\{B_1, B_2\}$ .

FIG 23. An example for the case  $\{A_1, B_1, C_1\}$ .



FIG 24. An example for the case  $\{A_1, B_1, B_2\}$ .

### 2.3. The case in which both $X$ and $Y$ have exactly two distinct eigenvalues

For this special case, we parameterize  $X$  and  $Y$  with  $a, b, c, d \in \mathbb{R}$  (not ordered), and a unit quaternion  $q = z + wj \in S_{\mathbb{H}}^3$ , where  $z, w \in \mathbb{C}$ ,  $|z|^2 + |w|^2 = 1$  as

$$X = U \begin{pmatrix} e^a & 0 & 0 \\ 0 & e^b & 0 \\ 0 & 0 & e^b \end{pmatrix} U^T, \quad Y = U\phi(q) \begin{pmatrix} e^c & 0 & 0 \\ 0 & e^d & 0 \\ 0 & 0 & e^d \end{pmatrix} (U\phi(q))^T \quad (17)$$

where  $U \in \text{SO}(3)$  and  $\phi : S_{\mathbb{H}}^3 \rightarrow \text{SO}(3)$  is the natural two-to-one Lie-group homomorphism. Without loss of generality, we assume  $\text{Re}(q) = \text{Re}(z) > 0$  so that  $\phi(q)$  is not an involution.

There are four different cases of MSSR curves arising from the parametrization of (17), as summarized in Table 3 of the main article. These cases are denoted by  $A'_1, A'_2, B'$  and  $C'$ . Our goal here is to illustrate these cases by providing representative examples. For this, we partially rewrite the conditions in Table 5 of the main article. First note that  $0 < |z| \leq 1$ ,  $0 \leq \cos^{-1}|z| < \frac{\pi}{2}$ ,  $|w| = \sqrt{1 - |z|^2} = \cos(\frac{\pi}{2} - \cos^{-1}|z|)$ , and

$$\begin{aligned} \varphi &= \cos^{-1}(\max\{|z|, |w|\}) \\ &= \min\{\cos^{-1}|z|, \cos^{-1}(\sqrt{1 - |z|^2})\} \\ &= \min\{\cos^{-1}|z|, \frac{\pi}{2} - \cos^{-1}|z|\} \\ &= \begin{cases} \cos^{-1}|z|, & 0 \leq \cos^{-1}|z| \leq \frac{\pi}{4}; \\ \frac{\pi}{2} - \cos^{-1}|z|, & \frac{\pi}{4} \leq \cos^{-1}|z| < \frac{\pi}{2}. \end{cases} \end{aligned} \quad (18)$$

From Theorem 4.4 of the main article,  $\ell_{\text{id}}^2 - \ell_{13}^2 = 2k\pi(\varphi - \frac{\pi}{8}) - 2(a - b)(c - d)$ . Let

$$m = \frac{2(a - b)(c - d)}{k\pi}.$$

Unlike in the  $\text{Sym}^+(2)$  case, this  $m$  can be either positive or negative, but not zero. If  $X$  and  $Y$  are both prolates (or both oblates), then  $m > 0$ . If  $X$  is an oblate and  $Y$  is a prolate (or vice versa), then  $m < 0$ . We have

$$\ell_{\text{id}} < \ell_{13} \iff m > 2(\varphi - \frac{\pi}{8}). \quad (19)$$

Moreover,

$$|z| > |w| \iff \frac{1}{\sqrt{2}} < |z| \leq 1 \iff 0 \leq \cos^{-1}|z| < \frac{\pi}{4} \quad (20)$$

$$|z| < |w| \iff 0 < |z| < \frac{1}{\sqrt{2}} \iff \frac{\pi}{4} < \cos^{-1}|z| < \frac{\pi}{2} \quad (21)$$

Combining (18)-(21), the conditions for the nine subcases in Table 5 of the main article are represented by  $m \neq 0$  and  $\cos^{-1}|z| \in [0, \frac{\pi}{2})$ , as shown in Fig. 25. These subcases can be sub-divided by the sign of  $m$ .

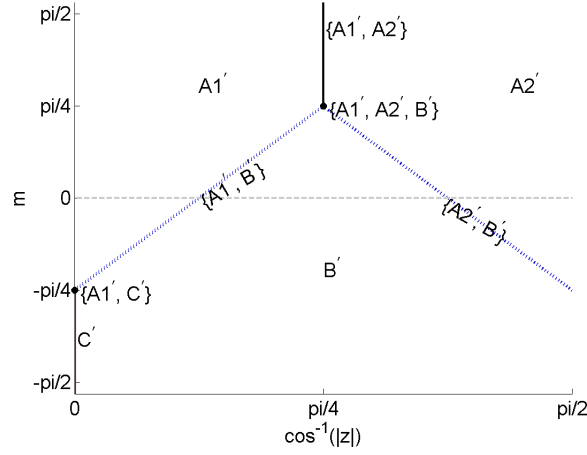


FIG 25. Unique and non-unique MSSR curves in  $Sym^+(3)$  when both  $X$  and  $Y$  have exactly two distinct eigenvalues: Schematic illustration for the seven (or nine) subcases. The horizontal line  $m = 0$  is excluded.

In the following we take a few representative examples of the nine subcases. Each example of MSSR curve  $\chi$  is accompanied by its shape-classification changes. Note that the seven subcases not involving  $C'$  resemble the seven subcases of  $p = 2$ . The case  $C'$  is only defined for  $|z| = 1$  (or  $\cos^{-1}|z| = 0$ ), in which situations the cases  $A'_2, B'_1$  are not defined. The list of these examples is given below, with the data  $(a, b, c, d) \in \mathbb{R}^4$  and  $q \in S^3_{\mathbb{H}} \subset \mathbb{R}^4$  to define  $X$  and  $Y$  in (17).

1.  $\{A'_1\}$ ,  $m > 0$ . Unique MSSR curve  $\chi$ . See Fig. 26. The shapes of  $\chi(t)$  are always prolate (or oblate) for all  $t \in [0, 1]$ . In Fig. 26, we have set  $(a, b, c, d) = (\frac{\pi}{\sqrt{8}} + 1, 1, \frac{\pi}{\sqrt{8}} + 3, 2)$ ,  $q = (0.8315, 0.4028, 0.3827, 0)$ .
2.  $\{A'_1\}$ ,  $m < 0$ . Unique MSSR curve. See Fig. 27. The shape-classification changes of the MSSR curve  $\chi(t)$  evaluated from  $t = 0$  to  $t = 1$  are either (oblate  $\rightarrow$  sphere  $\rightarrow$  prolate) or (prolate  $\rightarrow$  sphere  $\rightarrow$  oblate). In Fig. 27, we have set  $(a, b, c, d) = (0.9, 1, 0.5, 0.4)$ ,  $q = (0.8315, 0.5469, 0.0980, 0)$ .
3.  $\{B'\}$ . Unique MSSR curve. See Fig. 29. For prolate  $X$ , the shape-classification changes are (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate) if  $m > 0$ , (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate) if  $m < 0$ . For oblate  $X$ , interchange “oblate” and “prolate” in these shape-classification changes. In Fig. 29, we have set  $(a, b, c, d) = (2, 1, 1, 0.5)$ ,  $q = (0.3827, 0.5946, 0.7071, 0)$ .
4.  $\{A'_1, A'_2\}$ . Two MSSR curves with rotation angle  $\pi/2$ . See Fig. 28. The shape-changes are again dependent on the sign of  $m$ ; see items 1 and 2. In Fig. 28, we have set  $(a, b, c, d) = (1.5, 0.5, 2, 0.2)$ ,  $q = (0.3827, 0.5946, 0.7071, 0)$ .
5.  $\{A'_1, A'_2, B'\}$ . Three MSSR curves (two with rotation angle  $\pi/2$  and the other involving no rotation). See Fig. 30, in which we have set  $(a, b, c, d) = (\frac{\pi}{\sqrt{8}} + 1, 1, \frac{\pi}{\sqrt{8}} + 0.5, 0.5)$ ,  $q = (0.3827, 0.5946, 0.7071, 0)$ .

6.  $\{C'\}$ . Uncountably many MSSR curves. See Fig. 31. The set of MSSR curves is in natural one-to-one correspondence with  $S_{\mathbb{C}}^1$ . In this case  $m < 0$ , and the corresponding shape changes are the same as the case  $\{B'\}$ , with  $m < 0$ : (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate). In Fig. 31, we have set  $(a, b, c, d) = (2, 0, 1, 2)$ ,  $q = (1, 0, 0, 0)$ .

Note that in all examples above we have chosen  $z$  and  $w$  for a given  $|z|$  in the following way. If  $|z| = 1$  (equivalently,  $\cos^{-1}(|z|) = 0$ ), then  $w = 0$  and we have set  $z = 1 = q$ . For a given  $\varphi \in (0, \pi/4]$ , write  $z = z_1 + z_2 i$  (where  $z_1, z_2$  are real), and choose  $z_1$  such that  $0 < z_1 \leq \cos(\varphi)$ . Then,  $z_2 = \pm \sqrt{\cos(\varphi)^2 - z_1^2}$ , and in this case  $|z| \geq |w|$ . Finally we choose  $w$  by setting  $w = \sqrt{1 - |z|^2}$ . (The case  $|z| < |w|$  can be handled similarly.)

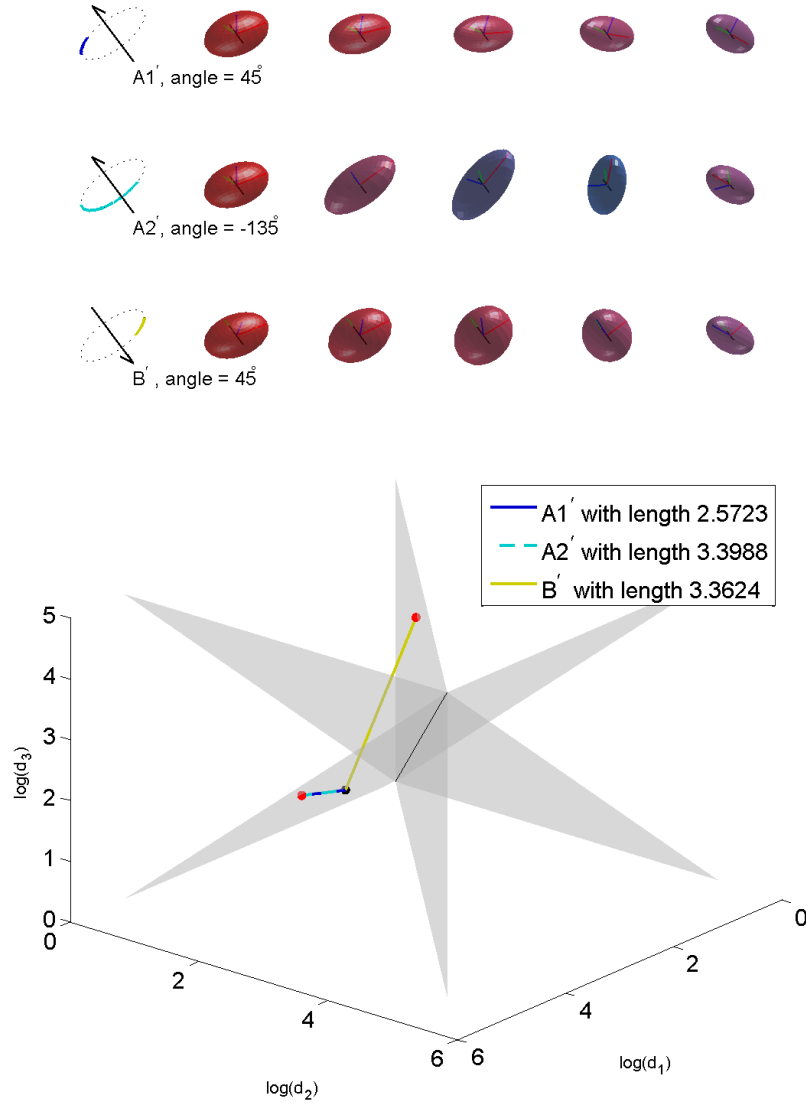


FIG 26. An example for the case  $\{A_1'\}$  (The scaling-rotation curve corresponding to  $A_1'$  is the unique MSSR curve.) Each of the cases  $A_1'$ ,  $A_2'$ , and  $B'$  represents the corresponding scaling-rotation curves defined in Table 3 of the main article, whose length can be found in the legend. Since the rotational degrees of freedom have been projected out in the bottom panel, the relative lengths of the straight-line segments do not accurately reflect the relative lengths of the curves. Note that  $m > 0$  in this example. The eigenvalue paths corresponding to  $A_1'$  and  $A_2'$  stay in a single connected component of  $\mathcal{D}_{J_1}$  (represented by one of the shaded open half-planes) and their shapes are all prolates (if both  $X$  and  $Y$  are prolates) or all oblates (if both  $X$  and  $Y$  are oblates). On the other hand, the eigenvalue path corresponding to  $B'$  travels through  $\mathcal{D}_{\text{top}}$  and another shaded plane corresponding to  $J_2$ . That is, the shape-classification changes are (prolate  $\rightarrow$  tri-axial  $\rightarrow$  oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate).

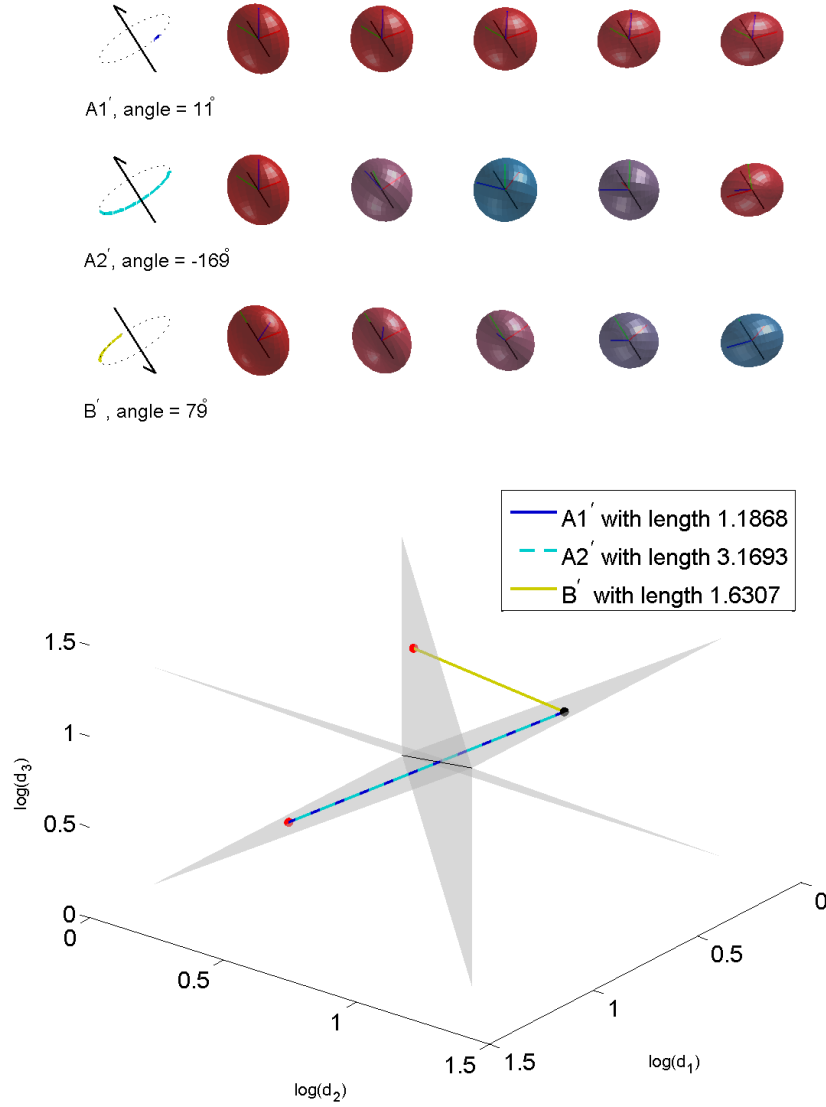


FIG 27. An example for the case  $\{A_1'\}$  but with  $m < 0$ . The eigenvalue paths corresponding to  $A_1'$  and  $A_2'$  stay in the shaded plane corresponding to  $\mathcal{D}_{J_1} \cup \mathcal{D}_{\text{bot}}$ , but they pass through  $\mathcal{D}_{\text{bot}}$ . The shape-classification changes from  $X$  to  $Y$  via  $A_1'$  or  $A_2'$  are (oblate  $\rightarrow$  sphere  $\rightarrow$  prolate). Similar to the case  $\{A_1'\}$  with  $m > 0$ , the eigenvalue path corresponding to  $B'$  travels through  $\mathcal{D}_{\text{top}}$ , but never intersects other shaded planes. The shape-classification changes are (oblate  $\rightarrow$  tri-axial  $\rightarrow$  prolate).

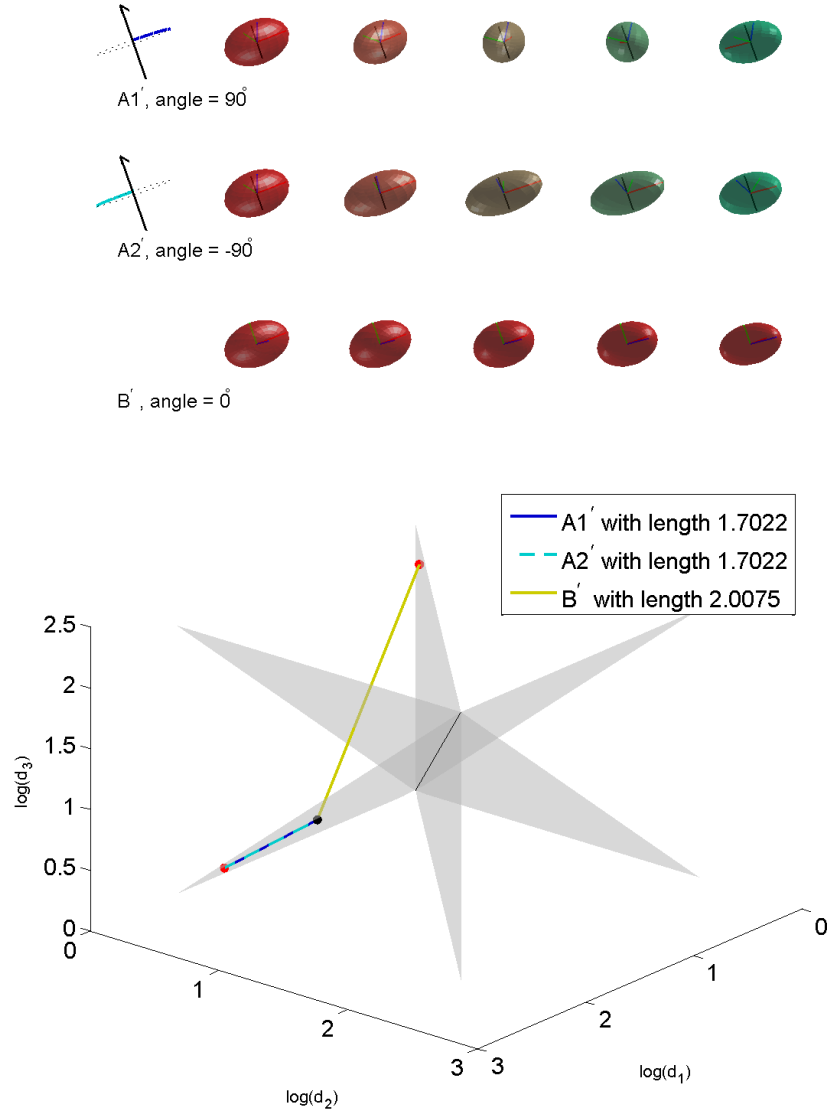


FIG 28. An example for the case  $\{A_1', A_2'\}$  with  $m > 0$ . The shape-classification changes along each of  $A_1'$ ,  $A_2'$  and  $B'$  again depend on the sign of  $m$ .

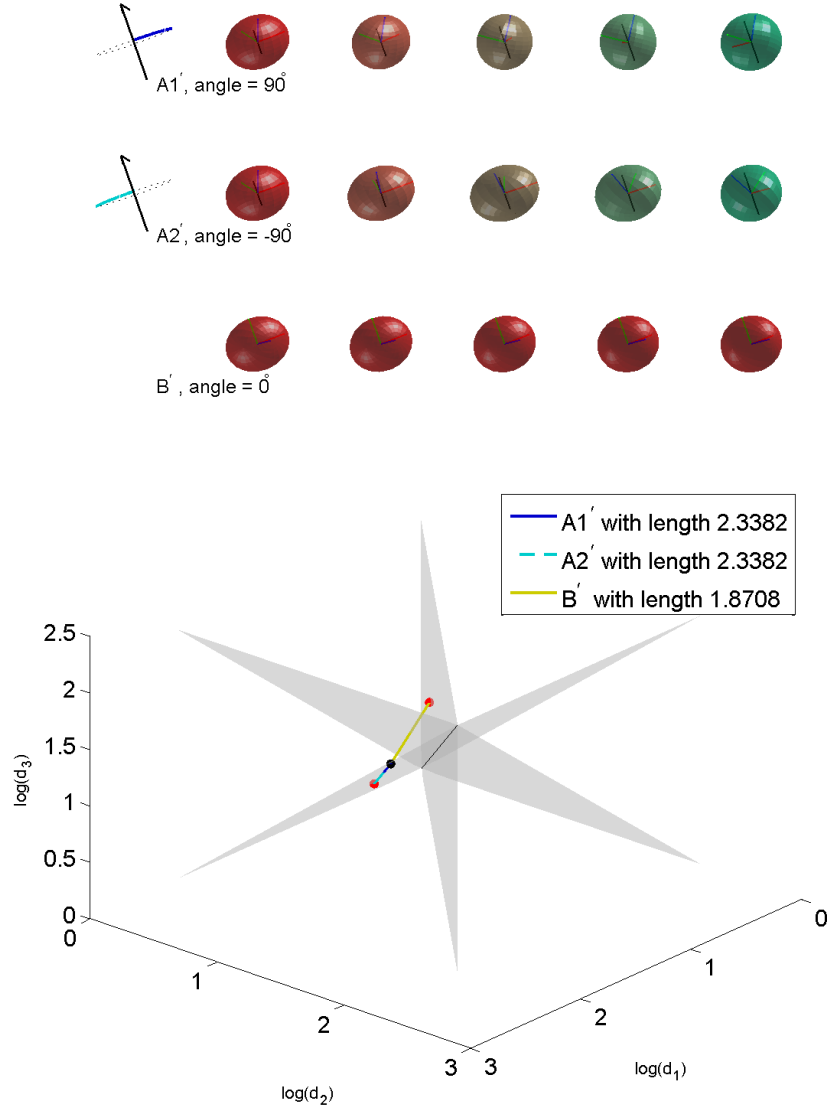
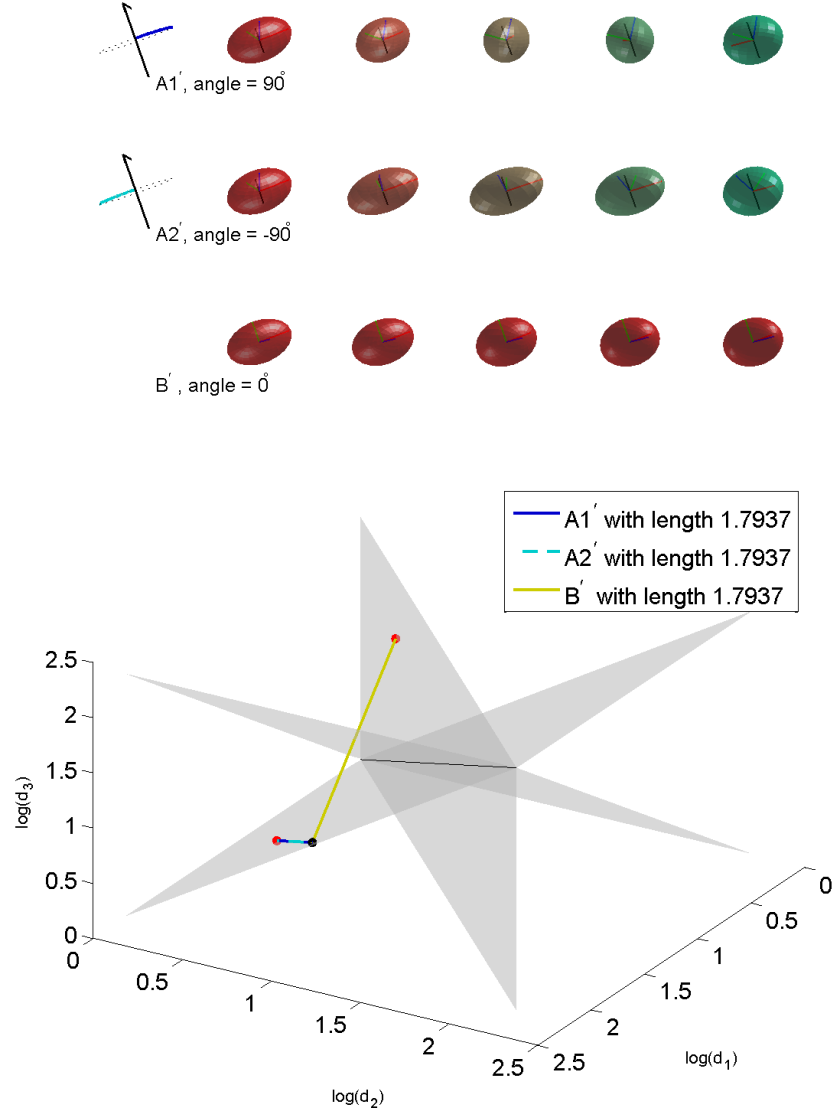


FIG 29. An example for the case  $\{B'\}$  with  $m > 0$ . The shape-classification changes along each of  $A_1'$ ,  $A_2'$  and  $B'$  again depend on the sign of  $m$ .



FIG 30. An example for the case  $\{A'_1, A'_2, B'\}$ .

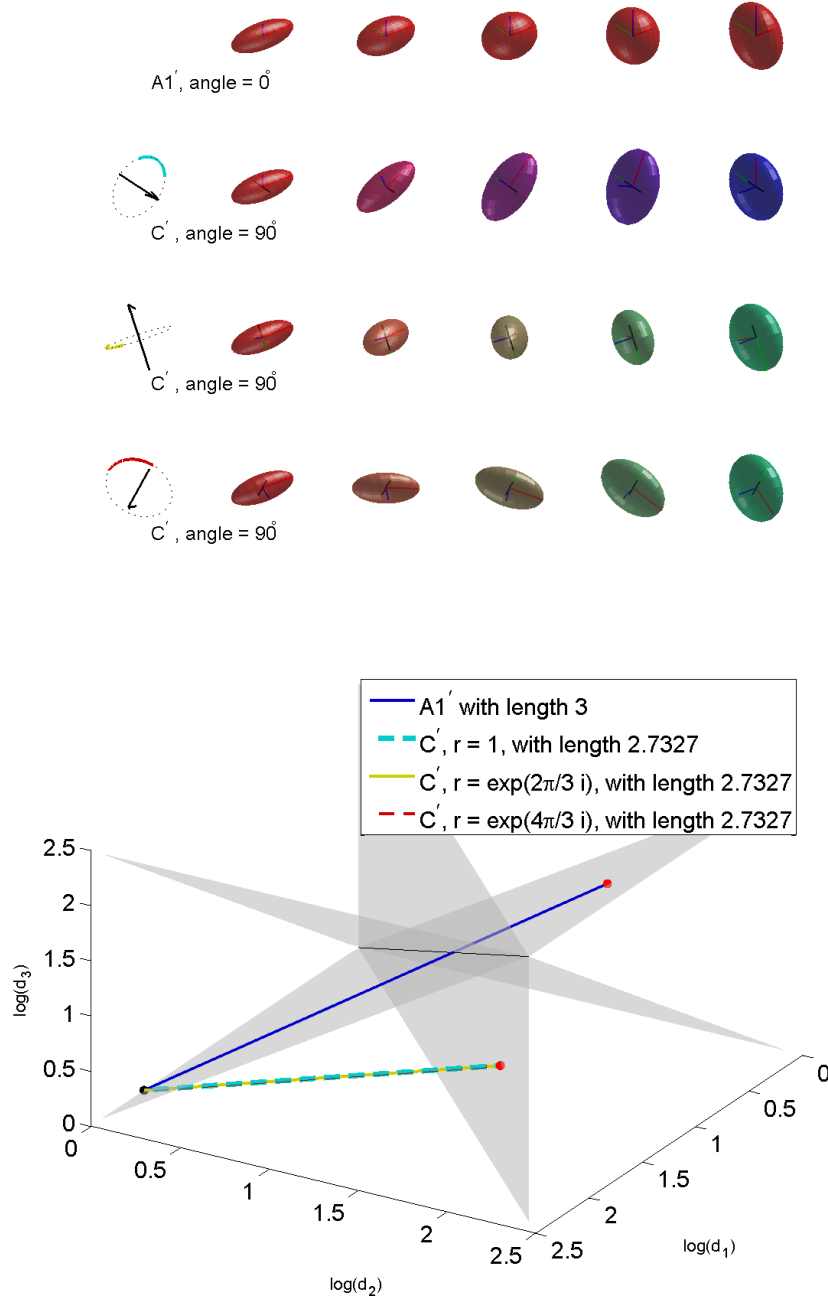


FIG 31. An example for the case  $\{C'\}$ . For each of the case  $C'$ , the rotation axis (depicted as the black line segment) is orthogonal to the (red) major semi-axis of  $X$ . It is shown in the proof of Theorem 5.3(i) that there is one-to-one correspondence between the “equator” of  $X$  and the family  $\mathcal{M}_{C'}$ ; see also Remark 5.5 of the main article.

## References

- [1] S. JUNG, A. SCHWARTZMAN, AND D. GROISSER, *Scaling-rotation distance and interpolation of symmetric positive definite matrix*, Siam J. Matrix Anal. Appl., 36 (2015), pp. 1180–1201.